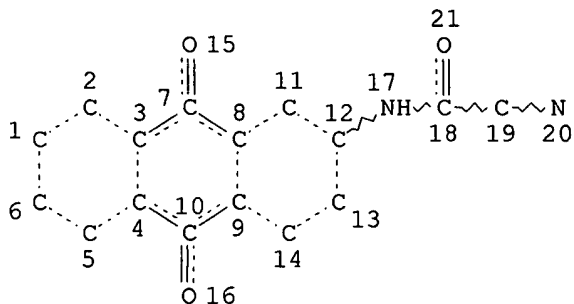


2 0 SEA SSS FUL L1
=> structure l1
ENTER (DIS), GRA, NOD, BON OR ?:nod 16 o, dis



ENTER (DIS), GRA, NOD, BON OR ?:end
L3 STRUCTURE CREATED

=> search l3 sss full
FULL SEARCH INITIATED 17:03:26 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 4541 TO ITERATE

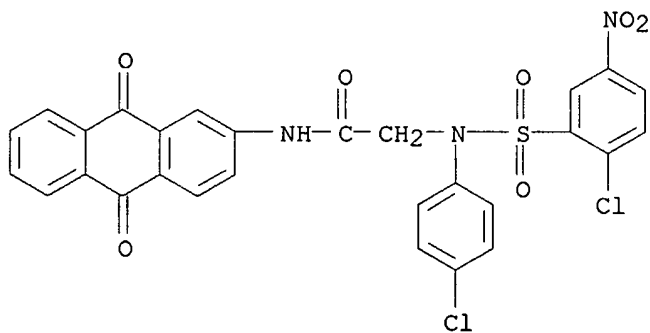
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47 ANSWERS

L4 47 SEA SSS FUL L3

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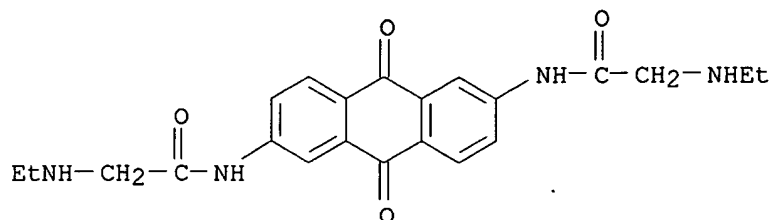
L4 ANSWER 1 OF 47 REGISTRY COPYRIGHT 2003 ACS
RN 509105-38-8 REGISTRY
CN Acetamide, 2-[[[(2-chloro-5-nitrophenyl)sulfonyl] (4-chlorophenyl)amino]-N-(9,10-dihydro-9,10-dioxo-2-anthracenyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C28 H17 Cl2 N3 O7 S
SR Chemical Library



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

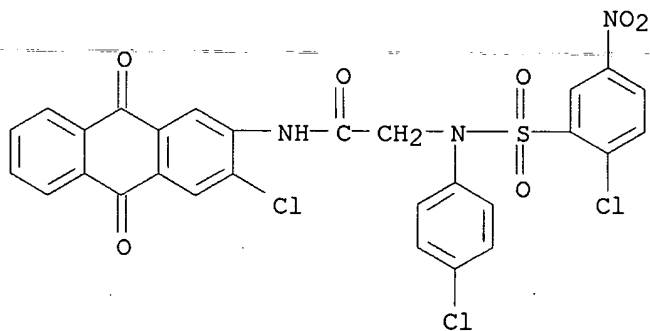
L4 ANSWER 2 OF 47 REGISTRY COPYRIGHT 2003 ACS
RN 500865-49-6 REGISTRY
CN Acetamide, N,N'-(9,10-dihydro-9,10-dioxo-2,6-anthracenediyl)bis[2-(ethylamino)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
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SR Chemical Library

L.N. 10/02244/
12/20
2001



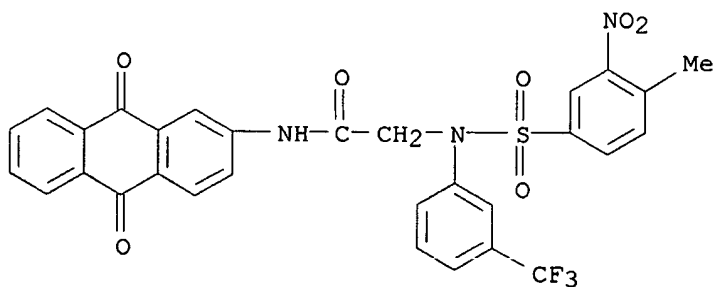
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L4 ANSWER 3 OF 47 REGISTRY COPYRIGHT 2003 ACS
 RN 482319-42-6 REGISTRY
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 FS 3D CONCORD
 MF C28 H16 Cl3 N3 O7 S
 SR Chemical Library
 LC STN Files: CHEMCATS



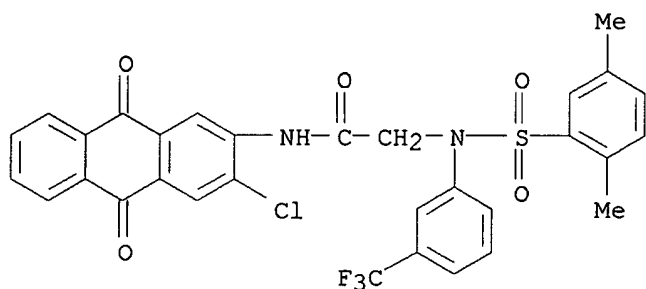
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 4 OF 47 REGISTRY COPYRIGHT 2003 ACS
 RN 481023-07-8 REGISTRY
 CN Acetamide, N-(9,10-dihydro-9,10-dioxo-2-anthracenyl)-2-[[3-(trifluoromethyl)phenyl]amino]- (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C30 H20 F3 N3 O7 S
 SR Chemical Library
 LC STN Files: CHEMCATS



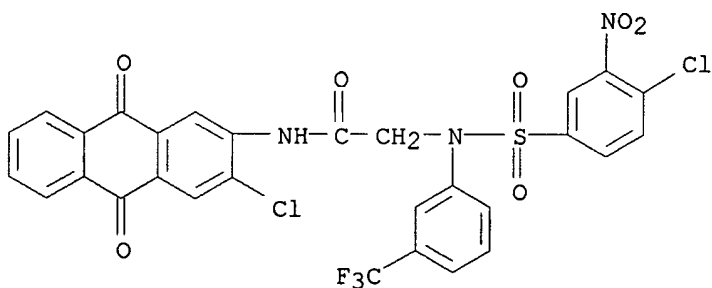
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 5 OF 47 REGISTRY COPYRIGHT 2003 ACS
RN 479715-40-7 REGISTRY
CN Acetamide, N-(3-chloro-9,10-dihydro-9,10-dioxo-2-anthracenyl)-2-[[(2,5-dimethylphenyl)sulfonyl][3-(trifluoromethyl)phenyl]amino]- (9CI) (CA INDEX NAME)
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SR Chemical Library
LC STN Files: CHEMCATS



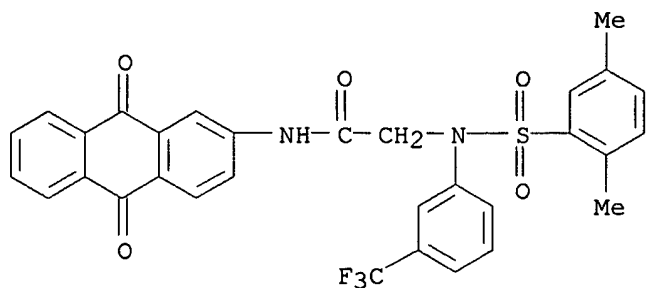
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L4 ANSWER 6 OF 47 REGISTRY COPYRIGHT 2003 ACS
RN 478862-07-6 REGISTRY
CN Acetamide, N-(3-chloro-9,10-dihydro-9,10-dioxo-2-anthracenyl)-2-[[(4-chloro-3-nitrophenyl)sulfonyl][3-(trifluoromethyl)phenyl]amino]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C29 H16 Cl2 F3 N3 O7 S
SR Chemical Library
LC STN Files: CHEMCATS



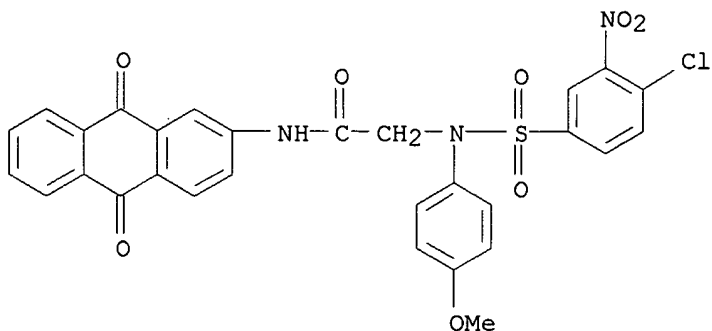
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 7 OF 47 REGISTRY COPYRIGHT 2003 ACS
RN 474690-02-3 REGISTRY
CN Acetamide, N-(9,10-dihydro-9,10-dioxo-2-anthracenyl)-2-[[(2,5-dimethylphenyl)sulfonyl][3-(trifluoromethyl)phenyl]amino]- (9CI) (CA INDEX NAME)
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SR Chemical Library
LC STN Files: CHEMCATS



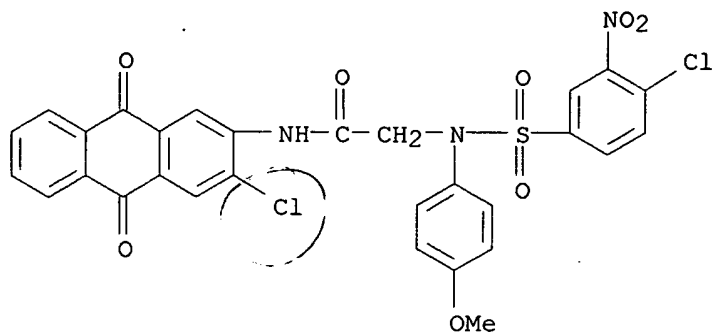
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L4 ANSWER 8 OF 47 REGISTRY COPYRIGHT 2003 ACS
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 FS 3D CONCORD
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 SR Chemical Library
 LC STN Files: CHEMCATS



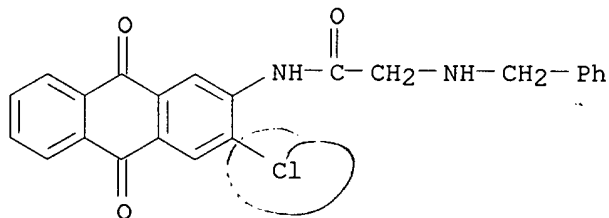
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L4 ANSWER 9 OF 47 REGISTRY COPYRIGHT 2003 ACS
 RN 473633-89-5 REGISTRY
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 FS 3D CONCORD
 MF C29 H19 Cl2 N3 O8 S
 SR Chemical Library
 LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 ANSWER 10 OF 47 REGISTRY COPYRIGHT 2003 ACS
 RN 225929-49-7 REGISTRY
 CN Acetamide, N-(3-chloro-9,10-dihydro-9,10-dioxo-2-anthracenyl)-2-
 [(phenylmethyl)amino]- (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C23 H17 Cl N2 O3
 SR CA
 LC STN Files: CA, CAPLUS

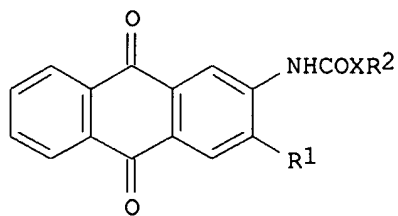


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

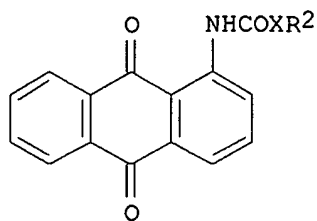
1 REFERENCES IN FILE CA (1957 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 131:5086 CA
 TI Synthesis and pharmacological properties of novel
 [(aminoacyl)amino]anthraquinones
 AU Litvinova, L. A.; Lyakhova, S. A.; Andronati, S. A.; Zhukova, N. A.;
 Yasinskaya, O. G.; Galkin, B. N.; Filippova, T. O.; Golovenko, N. Ya.
 CS Fiz.-Khim. Inst. im. A. V. Bogatskogo, Nats. Akad. Nauk Ukrainy, Odessa,
 Ukraine
 SO Khimiko-Farmatsevticheskii Zhurnal (1998), 32(12), 14-17
 CODEN: KHFZAN; ISSN: 0023-1134
 PB Izdatel'stvo Folium
 DT Journal
 LA Russian
 GI



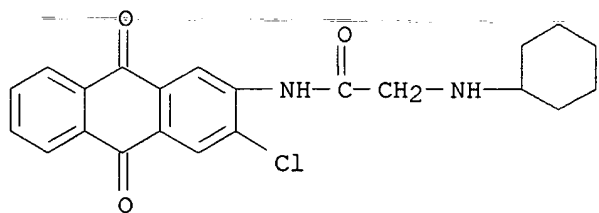
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II

AB Title compds. such as I (R1 = H, Cl; X = CH2, CH2CH2, CHMe; R2 = NHMe, NEt2, piperidino, morpholino) and II (same X, R2) were prepd. by N-(haloacylation) of 2- and 1-aminoanthraquinones, followed by amination. The products were tested for antiviral and antiemphysema (caused in mice by NO2 inhalation) activity.

L4 ANSWER 11 OF 47 REGISTRY COPYRIGHT 2003 ACS
 RN 225929-48-6 REGISTRY
 CN Acetamide, N-(3-chloro-9,10-dihydro-9,10-dioxo-2-anthracenyl)-2-(cyclohexylamino)- (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C22 H21 Cl N2 O3
 SR CA
 LC STN Files: CA, CAPLUS

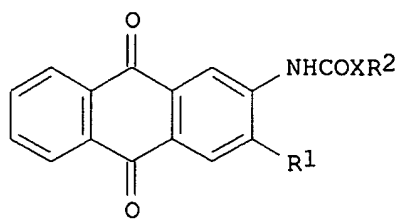


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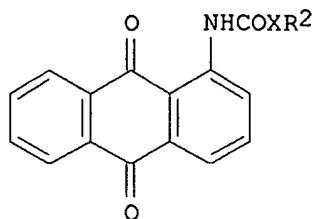
1 REFERENCES IN FILE CA (1957 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 131:5086 CA
 TI Synthesis and pharmacological properties of novel [(aminoacyl)amino]anthraquinones
 AU Litvinova, L. A.; Lyakhova, S. A.; Andronati, S. A.; Zhukova, N. A.; Yasinskaya, O. G.; Galkin, B. N.; Filippova, T. O.; Golovenko, N. Ya.
 CS Fiz.-Khim. Inst. im. A. V. Bogatskogo, Nats. Akad. Nauk Ukrainy, Odessa, Ukraine
 SO Khimiko-Farmatsevticheskii Zhurnal (1998), 32(12), 14-17
 CODEN: KHFZAN; ISSN: 0023-1134
 PB Izdatel'stvo Folium
 DT Journal
 LA Russian
 GI



I



II

AB Title compds. such as I (R1 = H, Cl; X = CH2, CH2CH2, CHMe; R2 = NHMe, NEt2, piperidino, morpholino) and II (same X, R2) were prepd. by N-(haloacylation) of 2- and 1-aminoanthraquinones, followed by amination. The products were tested for antiviral and antiemphysema (caused in mice by NO2 inhalation) activity.

L4 ANSWER 12 OF 47 REGISTRY COPYRIGHT 2003 ACS

RN 225929-47-5 REGISTRY

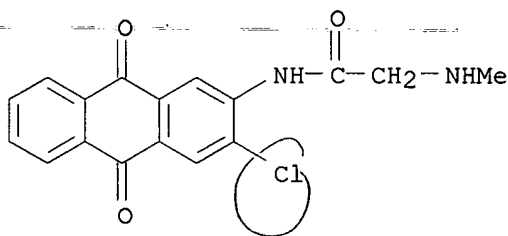
CN Acetamide, N-(3-chloro-9,10-dihydro-9,10-dioxo-2-anthracenyl)-2-(methylamino)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C17 H13 Cl N2 O3

SR CA

LC STN Files: CA, CAPLUS, CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)

1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 131:5086 CA

TI Synthesis and pharmacological properties of novel [(aminoacyl)amino]anthraquinones

AU Litvinova, L. A.; Lyakhova, S. A.; Andronati, S. A.; Zhukova, N. A.; Yasinskaya, O. G.; Galkin, B. N.; Filippova, T. O.; Golovenko, N. Ya.

CS Fiz.-Khim. Inst. im. A. V. Bogatskogo, Nats. Akad. Nauk Ukrainy, Odessa, Ukraine

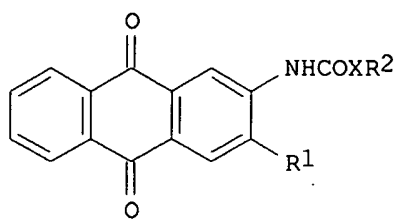
SO Khimiko-Farmatsevticheskii Zhurnal (1998), 32(12), 14-17
CODEN: KHFZAN; ISSN: 0023-1134

PB Izdatel'stvo Folium

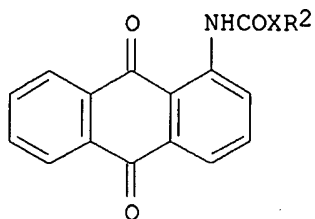
DT Journal

LA Russian

GI



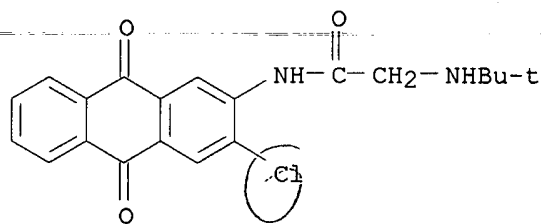
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AB Title compds. such as I (R1 = H, Cl; X = CH2, CH2CH2, CHMe; R2 = NHMe, NEt2, piperidino, morpholino) and II (same X, R2) were prepd. by N-(haloacylation) of 2- and 1-aminoanthraquinones, followed by amination. The products were tested for antiviral and antiemphysema (caused in mice by NO2 inhalation) activity.

L4 ANSWER 13 OF 47 REGISTRY COPYRIGHT 2003 ACS
 RN 225929-46-4 REGISTRY
 CN Acetamide, N-(3-chloro-9,10-dihydro-9,10-dioxo-2-anthracenyl)-2-[(1,1-dimethylethyl)amino]- (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C20 H19 Cl N2 O3
 SR CA
 LC STN Files: CA, CAPLUS

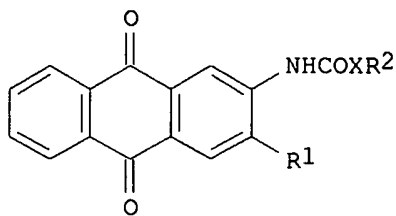


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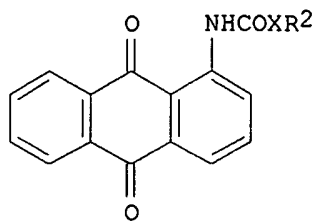
1 REFERENCES IN FILE CA (1957 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 131:5086 CA
 TI Synthesis and pharmacological properties of novel [(aminoacyl)amino]anthraquinones
 AU Litvinova, L. A.; Lyakhova, S. A.; Andronati, S. A.; Zhukova, N. A.; Yasinskaya, O. G.; Galkin, B. N.; Filippova, T. O.; Golovenko, N. Ya.
 CS Fiz.-Khim. Inst. im. A. V. Bogatskogo, Nats. Akad. Nauk Ukrainy, Odessa, Ukraine
 SO Khimiko-Farmatsevticheskii Zhurnal (1998), 32(12), 14-17
 CODEN: KHFZAN; ISSN: 0023-1134
 PB Izdatel'stvo Folium
 DT Journal
 LA Russian
 GI



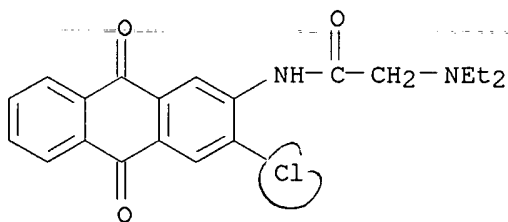
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II

AB Title compds. such as I (R1 = H, Cl; X = CH2, CH2CH2, CHMe; R2 = NHMe, NEt2, piperidino, morpholino) and II (same X, R2) were prepd. by N-(haloacylation) of 2- and 1-aminoanthraquinones, followed by amination. The products were tested for antiviral and antiemphysema (caused in mice by NO2 inhalation) activity.

L4 ANSWER 14 OF 47 REGISTRY COPYRIGHT 2003 ACS
 RN 225929-43-1 REGISTRY
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 FS 3D CONCORD
 MF C20 H19 Cl N2 O3
 SR CA
 LC STN Files: CA, CAPLUS

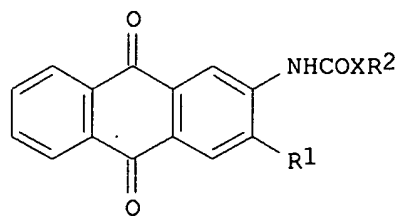


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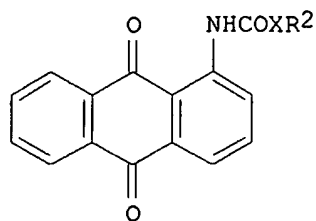
1 REFERENCES IN FILE CA (1957 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 131:5086 CA
 TI Synthesis and pharmacological properties of novel [(aminoacyl)amino]anthraquinones
 AU Litvinova, L. A.; Lyakhova, S. A.; Andronati, S. A.; Zhukova, N. A.; Yasinskaya, O. G.; Galkin, B. N.; Filippova, T. O.; Golovenko, N. Ya.
 CS Fiz.-Khim. Inst. im. A. V. Bogatskogo, Nats. Akad. Nauk Ukrainy, Odessa, Ukraine
 SO Khimiko-Farmatsevticheskii Zhurnal (1998), 32(12), 14-17
 CODEN: KHFZAN; ISSN: 0023-1134
 PB Izdatel'stvo Folium
 DT Journal
 LA Russian
 GI



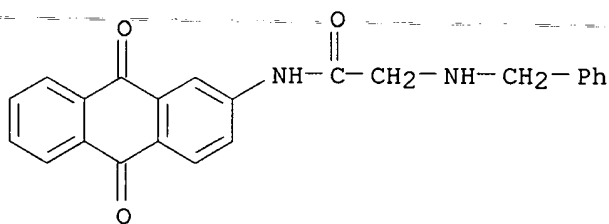
I



II

AB Title compds. such as I (R1 = H, Cl; X = CH2, CH2CH2, CHMe; R2 = NHMe, NEt2, piperidino, morpholino) and II (same X, R2) were prepd. by N-(haloacylation) of 2- and 1-aminoanthraquinones, followed by amination. The products were tested for antiviral and antiemphysema (caused in mice by NO2 inhalation) activity.

L4 ANSWER 15 OF 47 REGISTRY COPYRIGHT 2003 ACS
 RN 225929-42-0 REGISTRY
 CN Acetamide, N-(9,10-dihydro-9,10-dioxo-2-anthracenyl)-2-
 [(phenylmethyl)amino]- (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C23 H18 N2 O3
 SR CA
 LC STN Files: CA, CAPLUS

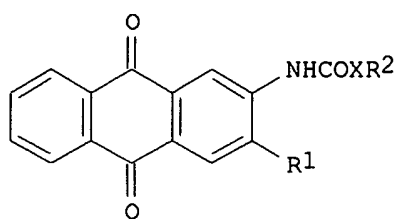


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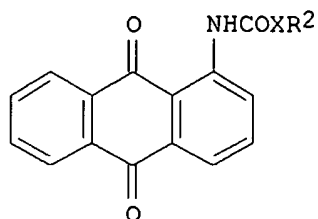
1 REFERENCES IN FILE CA (1957 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 131:5086 CA
 TI Synthesis and pharmacological properties of novel
 [(aminoacyl)amino]anthraquinones
 AU Litvinova, L. A.; Lyakhova, S. A.; Andronati, S. A.; Zhukova, N. A.;
 Yasinskaya, O. G.; Galkin, B. N.; Filippova, T. O.; Golovenko, N. Ya.
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 SO Khimiko-Farmatsevticheskii Zhurnal (1998), 32(12), 14-17
 CODEN: KHFZAN; ISSN: 0023-1134
 PB Izdatel'stvo Folium
 DT Journal
 LA Russian
 GI



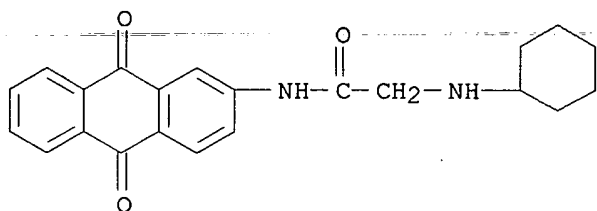
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II

AB Title compds. such as I (R1 = H, Cl; X = CH2, CH2CH2, CHMe; R2 = NHMe, NEt2, piperidino, morpholino) and II (same X, R2) were prepd. by N-(haloacylation) of 2- and 1-aminoanthraquinones, followed by amination. The products were tested for antiviral and antiemphysema (caused in mice by NO2 inhalation) activity.

L4 ANSWER 16 OF 47 REGISTRY COPYRIGHT 2003 ACS
 RN 225929-40-8 REGISTRY
 CN Acetamide, 2-(cyclohexylamino)-N-(9,10-dihydro-9,10-dioxo-2-anthracenyl)-(9CI) (CA INDEX NAME)
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 SR CA
 LC STN Files: CA, CAPLUS, CHEMCATS

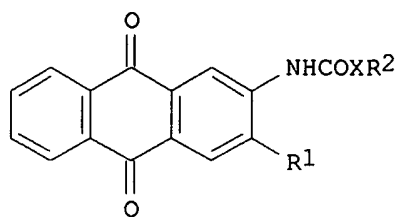


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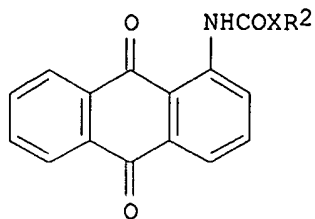
1 REFERENCES IN FILE CA (1957 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 131:5086 CA
 TI Synthesis and pharmacological properties of novel [(aminoacyl)amino]anthraquinones
 AU Litvinova, L. A.; Lyakhova, S. A.; Andronati, S. A.; Zhukova, N. A.; Yasinskaya, O. G.; Galkin, B. N.; Filippova, T. O.; Golovenko, N. Ya.
 CS Fiz.-Khim. Inst. im. A. V. Bogatskogo, Nats. Akad. Nauk Ukrainy, Odessa, Ukraine
 SO Khimiko-Farmatsevticheskii Zhurnal (1998), 32(12), 14-17
 CODEN: KHFZAN; ISSN: 0023-1134
 PB Izdatel'stvo Folium
 DT Journal
 LA Russian
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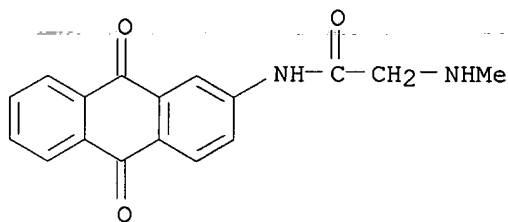
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II

AB Title compds. such as I (R1 = H, Cl; X = CH2, CH2CH2, CHMe; R2 = NHMe, NEt2, piperidino, morpholino) and II (same X, R2) were prepd. by N-(haloacylation) of 2- and 1-aminoanthraquinones, followed by amination. The products were tested for antiviral and antiemphysema (caused in mice by NO2 inhalation) activity.

L4 ANSWER 17 OF 47 REGISTRY COPYRIGHT 2003 ACS
 RN 225929-39-5 REGISTRY
 CN Acetamide, N-(9,10-dihydro-9,10-dioxo-2-anthracenyl)-2-(methylamino)-
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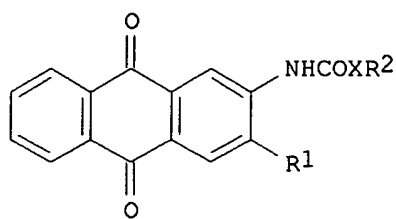


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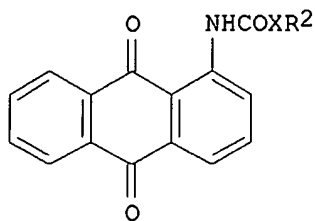
1 REFERENCES IN FILE CA (1957 TO DATE)
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REFERENCE 1

AN 131:5086 CA
 TI Synthesis and pharmacological properties of novel
 [(aminoacyl)amino]anthraquinones
 AU Litvinova, L. A.; Lyakhova, S. A.; Andronati, S. A.; Zhukova, N. A.;
 Yasinskaya, O. G.; Galkin, B. N.; Filippova, T. O.; Golovenko, N. Ya.
 CS Fiz.-Khim. Inst. im. A. V. Bogatskogo, Nats. Akad. Nauk Ukrainy, Odessa,
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 PB Izdatel'stvo Folium
 DT Journal
 LA Russian
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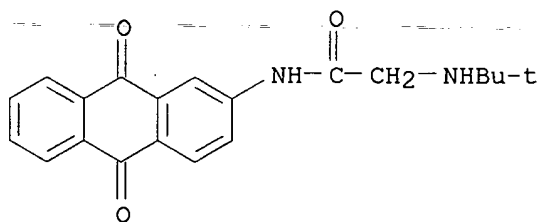
I



II

AB Title compds. such as I (R1 = H, Cl; X = CH2, CH2CH2, CHMe; R2 = NHMe, NEt2, piperidino, morpholino) and II (same X, R2) were prepd. by N-(haloacylation) of 2- and 1-aminoanthraquinones, followed by amination. The products were tested for antiviral and antiemphysema (caused in mice by NO2 inhalation) activity.

L4 ANSWER 18 OF 47 REGISTRY COPYRIGHT 2003 ACS
 RN 225929-38-4 REGISTRY
 CN Acetamide, N-(9,10-dihydro-9,10-dioxo-2-anthracenyl)-2-[(1,1-dimethylethyl)amino]- (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C20 H20 N2 O3
 SR CA
 LC STN Files: CA, CAPLUS



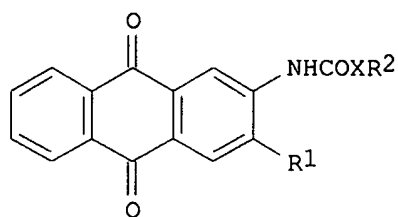
102

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

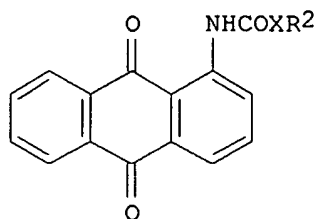
1 REFERENCES IN FILE CA (1957 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 131:5086 CA
 TI Synthesis and pharmacological properties of novel [(aminoacyl)amino]anthraquinones
 AU Litvinova, L. A.; Lyakhova, S. A.; Andronati, S. A.; Zhukova, N. A.; Yasinskaya, O. G.; Galkin, B. N.; Filippova, T. O.; Golovenko, N. Ya.
 CS Fiz.-Khim. Inst. im. A. V. Bogatskogo, Nats. Akad. Nauk Ukrainy, Odessa, Ukraine
 SO Khimiko-Farmatsevticheskii Zhurnal (1998), 32(12), 14-17
 CODEN: KHFZAN; ISSN: 0023-1134
 PB Izdatel'stvo Folium
 DT Journal
 LA Russian
 GI



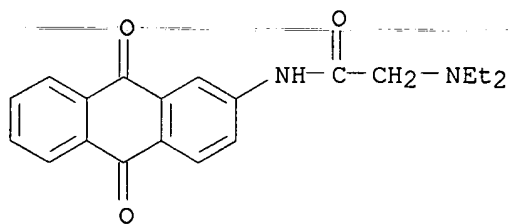
I



II

AB Title compds. such as I (R1 = H, Cl; X = CH2, CH2CH2, CHMe; R2 = NHMe, NEt2, piperidino, morpholino) and II (same X, R2) were prepd. by N-(haloacylation) of 2- and 1-aminoanthraquinones, followed by amination. The products were tested for antiviral and antiemphysema (caused in mice by NO2 inhalation) activity.

L4 ANSWER 19 OF 47 REGISTRY COPYRIGHT 2003 ACS
 RN 225929-33-9 REGISTRY
 CN Acetamide, 2-(diethylamino)-N-(9,10-dihydro-9,10-dioxo-2-anthracenyl)-
 (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C20 H20 N2 O3
 SR CA
 LC STN Files: CA, CAPLUS

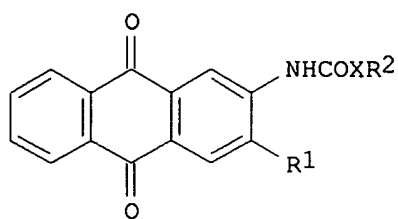


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

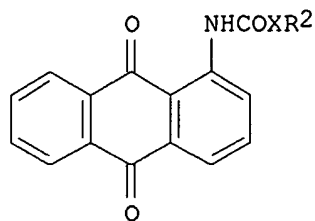
1 REFERENCES IN FILE CA (1957 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 131:5086 CA
 TI Synthesis and pharmacological properties of novel
 [(aminoacyl)amino]anthraquinones
 AU Litvinova, L. A.; Lyakhova, S. A.; Andronati, S. A.; Zhukova, N. A.;
 Yasinskaya, O. G.; Galkin, B. N.; Filippova, T. O.; Golovenko, N. Ya.
 CS Fiz.-Khim. Inst. im. A. V. Bogatskogo, Nats. Akad. Nauk Ukrainy, Odessa,
 Ukraine
 SO Khimiko-Farmatsevticheskii Zhurnal (1998), 32(12), 14-17
 CODEN: KHFZAN; ISSN: 0023-1134
 PB Izdatel'stvo Folium
 DT Journal
 LA Russian
 GI



I

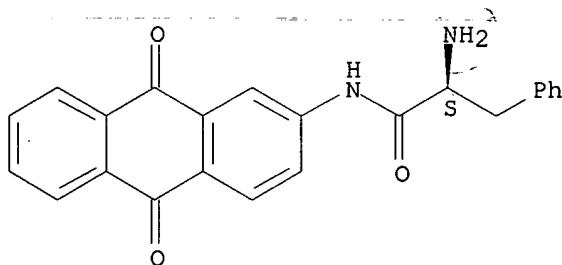


II

AB Title compds. such as I (R1 = H, Cl; X = CH2, CH2CH2, CHMe; R2 = NHMe, NEt2, piperidino, morpholino) and II (same X, R2) were prepd. by N-(haloacylation) of 2- and 1-aminoanthraquinones, followed by amination. The products were tested for antiviral and antiemphysema (caused in mice by NO2 inhalation) activity.

L4 ANSWER 20 OF 47 REGISTRY COPYRIGHT 2003 ACS
 RN 220037-50-3 REGISTRY
 CN Benzenepropanamide, .alpha.-amino-N-(9,10-dihydro-9,10-dioxo-2-anthracenyl)-, (.alpha.S)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C23 H18 N2 O3
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1957 TO DATE)
 2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 2 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 130:261201 CA
 TI On-bead combinatorial approach to the design of chiral stationary phases for HPLC
 AU Murer, Peter; Lewandowski, Kevin; Svec, Frantisek; Frechet, Jean M. J.
 CS Department of Chemistry, University of California, Berkeley, CA, 94720-1460, USA
 SO Analytical Chemistry (1999), 71(7), 1278-1284
 CODEN: ANCHAM; ISSN: 0003-2700
 PB American Chemical Society
 DT Journal
 LA English
 AB A library of 36 L-amino acid anilides, which are potential selectors for chiral HPLC, was synthesized in soln. and attached to functionalized macroporous polymer beads. The best selector from the library was identified by a deconvolution process using the HPLC sepn. of several racemic N-(3,5-dinitrobenzoyl)-.alpha.-amino acid alkylamides as a probe. In each deconvolution step, chiral stationary phases (CSPs) contg. a subset of the amino acid anilide selector library were screened for enantioselectivity. After the best CSP was chosen, the library was

further deconvoluted until the single best selector was found. The highest selectivity was obtained with a L-proline-1-indan anilide that exhibited .alpha. values up to 23 under normal-phase HPLC conditions. Six CSPs were prepd. using individual selectors from the library, and screening results indicate that the deconvolution process indeed led to the most selective receptor.

RE.CNT 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

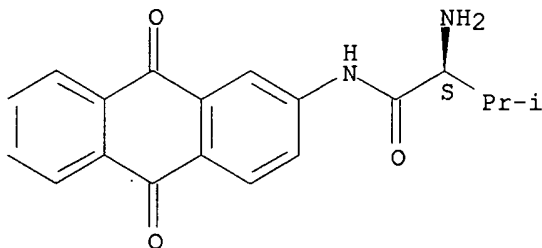
REFERENCE 2

AN 130:148000 CA
TI Combinatorial 'library on bead' approach to polymeric materials with vastly enhanced chiral recognition
AU Murer, Peter; Lewandowski, Kevin; Svec, Frantisek; Frechet, Jean M. J.
CS Department of Chemistry, University of California, Berkeley, CA, 94720-1460, USA
SO Chemical Communications (Cambridge) (1998), (23), 2559-2560
CODEN: CHCOFS; ISSN: 1359-7345
PB Royal Society of Chemistry
DT Journal
LA English
AB A general screening method for enantiomer recognition is introduced for the rapid prepn. of novel chiral stationary phases for HPLC in which libraries of mixed chiral selectors are immobilized on polymer beads and the resulting chiral phases tested in the sepn. of racemic targets followed by deconvolution to afford an optimized sepn. medium.

RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 21 OF 47 REGISTRY COPYRIGHT 2003 ACS
RN 220037-28-5 REGISTRY
CN Butanamide, 2-amino-N-(9,10-dihydro-9,10-dioxo-2-anthracenyl)-3-methyl-, (2S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C19 H18 N2 O3
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1957 TO DATE)
2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
2 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 130:261201 CA
TI On-bead combinatorial approach to the design of chiral stationary phases for HPLC
AU Murer, Peter; Lewandowski, Kevin; Svec, Frantisek; Frechet, Jean M. J.
CS Department of Chemistry, University of California, Berkeley, CA, 94720-1460, USA

SO Analytical Chemistry (1999), 71(7), 1278-1284

CODEN: ANCHAM; ISSN: 0003-2700

PB American Chemical Society

DT Journal

LA English

AB A library of 36 L-amino acid anilides, which are potential selectors for chiral HPLC, was synthesized in soln. and attached to functionalized macroporous polymer beads. The best selector from the library was identified by a deconvolution process using the HPLC sepn. of several racemic N-(3,5-dinitrobenzoyl)-.alpha.-amino acid alkylamides as a probe. In each deconvolution step, chiral stationary phases (CSPs) contg. a subset of the amino acid anilide selector library were screened for enantioselectivity. After the best CSP was chosen, the library was further deconvoluted until the single best selector was found. The highest selectivity was obtained with a L-proline-1-indan anilide that exhibited .alpha. values up to 23 under normal-phase HPLC conditions. Six CSPs were prepd. using individual selectors from the library, and screening results indicate that the deconvolution process indeed led to the most selective receptor.

RE.CNT 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 2

AN 130:148000 CA

TI Combinatorial 'library on bead' approach to polymeric materials with vastly enhanced chiral recognition

AU Murer, Peter; Lewandowski, Kevin; Svec, Frantisek; Frechet, Jean M. J.

CS Department of Chemistry, University of California, Berkeley, CA, 94720-1460, USA

SO Chemical Communications (Cambridge) (1998), (23), 2559-2560

CODEN: CHCOFS; ISSN: 1359-7345

PB Royal Society of Chemistry

DT Journal

LA English

AB A general screening method for enantiomer recognition is introduced for the rapid prepn. of novel chiral stationary phases for HPLC in which libraries of mixed chiral selectors are immobilized on polymer beads and the resulting chiral phases tested in the sepn. of racemic targets followed by deconvolution to afford an optimized sepn. medium.

RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 22 OF 47 REGISTRY COPYRIGHT 2003 ACS

RN 209247-79-0 REGISTRY

CN Acetamide, N,N'-(9,10-dihydro-9,10-dioxo-2,6-anthracenediyl)bis[2-[bis(2-hydroxyethyl)amino]- (9CI) (CA INDEX NAME)

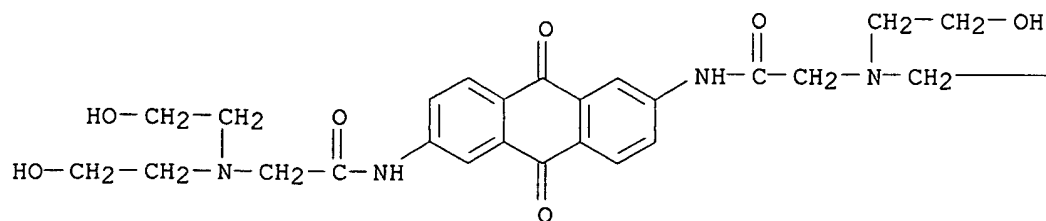
FS 3D CONCORD

MF C26 H32 N4 O8

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

PAGE 1-A



—CH₂—OH

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

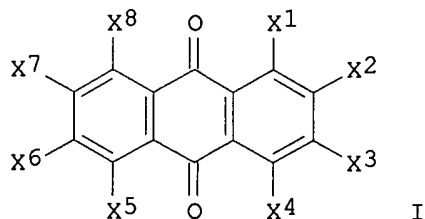
1 REFERENCES IN FILE CA (1957 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 129:81594 CA
 TI Preparation of anthraquinones as telomerase inhibitors
 IN Neidle, Stephen; Jenkins, Terence Charles; Hurley, Laurence Harold; Perry, Philip John
 PA Cancer Research Campaign Technology Ltd., UK; The Board of Regents, the University of Texas System; Neidle, Stephen; Jenkins, Terence Charles; Hurley, Laurence Harold; Perry, Philip John
 SO PCT Int. Appl., 75 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9825885	A1	19980618	WO 1997-GB3446	19971215
	W:		AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM		
	RW:		GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG		
	AU 9878468	A1	19980703	AU 1998-78468	19971215
PRAI	GB 1996-25941		19961213		
	WO 1997-GB3446		19971215		

GI

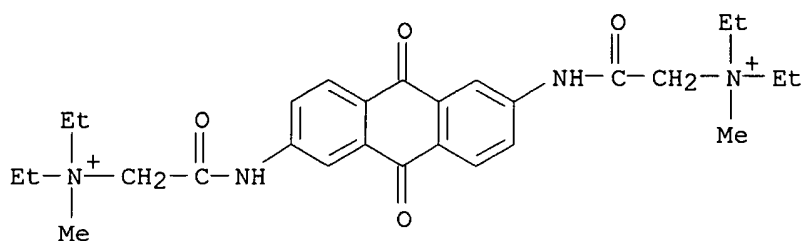


AB The title compds. [I; X1, X4 = HNCO(CH₂)_nNR₁R₂ (wherein R₁, R₂ = (un)substituted alkyl; NR₁R₂ = (un)substituted heterocyclyl; n = 1-6); X₂, X₃, X₅-X₈ = H, (un)substituted alkyl, halo] and their pharmaceutically acceptable acid addn. salts or quaternary ammonium salts, useful in the inhibition of telomerase activity and/or in the treatment of cancer, were prepd. Thus, reaction of 2-piperidinemethanol with 1,4-bis(3-chloropropionamido)anthracene-9,10-dione in EtOH followed by treatment of the resulting 1,4-bis[3-(2-hydroxymethyl-1-piperidino)propionamido]anthracene-9,10-dione with MeI afforded bisquaternary dimethiodide of I [X₁ = X₂ = 3-(2-hydroxymethyl-1-piperidino)propionamido; X₂, X₃, X₅-X₈ = H] which showed 100% telomerase inhibition at 50 .mu.M.

RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 23 OF 47 REGISTRY COPYRIGHT 2003 ACS
 RN 134888-29-2 REGISTRY
 CN Ethanaminium, 2,2'-[(9,10-dihydro-9,10-dioxo-2,6-anthracenediyl)diimino]bis[N,N-diethyl-N-methyl-2-oxo-, diiodide (9CI)
 (CA INDEX NAME)
 DR 139689-63-7
 MF C28 H38 N4 O4 . 2 I
 SR CA
 LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
 (*File contains numerically searchable property data)

● 2 I⁻

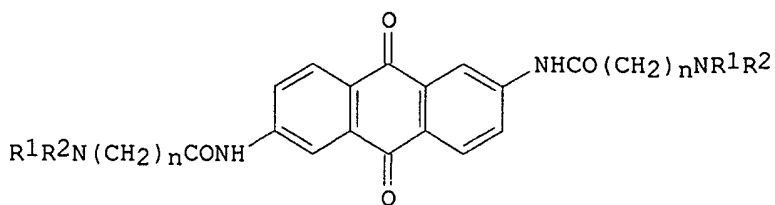
1 REFERENCES IN FILE CA (1957 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 115:49153 CA
 TI Preparation of 2,6-bis(aminoalkanoylamino)anthracene-9,10-diones as
 intercalating agents
 IN Neidle, Stephen; Jenkins, Terence Charles; Agbandje, Mavis
 PA Cancer Research Technology Ltd., UK
 SO PCT Int. Appl., 52 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9100265	A1	19910110	WO 1990-GB1004	19900629
	W: JP, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, IT, LU, NL, SE				
	EP 482119	A1	19920429	EP 1990-917804	19900629
	R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, LU, NL, SE				
PRAI	GB 1989-15028		19890630		
	WO 1990-GB1004		19900629		

GI

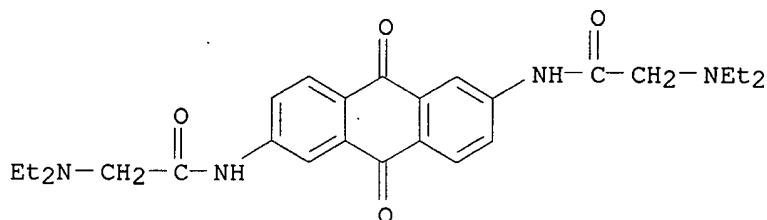


AB The title compds. [I; n = 1, 2, 3; R1, R2 = Et, CH₂CH₂OH, CH₂OH; or R1R2N = piperidino, 2- or 4-(2-hydroxyethyl)piperidino, 2-(hydroxymethyl)piperidino, 4-(2-hydroxyethyl)- or 4-methylpiperidino, morpholino], useful for treating a host suffering from cancer, are prepd. I intercalating into DNA with one side-chain of the mol. residing in each DNA groove, are cytotoxic and non-mutagenic. Thus, a suspension of 14.3 mmol 2,6-bis(3-chloropropionamido)anthracene-9,10-dione in EtOH was gently refluxed and 0.12 mol 4-(2-hydroxyethyl)piperidine in EtOH was added dropwise during 30 min and refluxing was continued for 5 h to give I [n = 2, R1R2N = 4-(2-hydroxyethyl)piperidino] (II). I stabilized various DNA's towards thermal denaturation, the effect of increasing the melting temp. for the DNA by I (n = 2) was comparable to that of mitoxantrone (III) (a known intercalator), and unwinded covalently-colored supercoiled plasmid PM2 DNA. I in vitro showed IC₅₀ of 0.25 - >100 .mu.mol/dm³ against L1210 leukemia cell lines, vs. 0.002 .mu.mol/dm³ with III. II.2AcOH at 200 mg/kg/day i.p. on days 3, 5, 6, and 7 increased 136.8% the life span of mice bearing L1210 leukemia tumor.

L4 ANSWER 24 OF 47 REGISTRY COPYRIGHT 2003 ACS
RN 134888-28-1 REGISTRY
CN Acetamide, N,N'-(9,10-dihydro-9,10-dioxo-2,6-anthracenediyl)bis[2-(diethylamino)-, diacetate (9CI) (CA INDEX NAME)
MF C26 H32 N4 O4 . 2 C2 H4 O2
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)

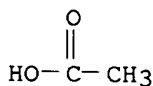
CM 1

CRN 72966-57-5
CMF C26 H32 N4 O4



CM 2

CRN 64-19-7
CMF C2 H4 O2

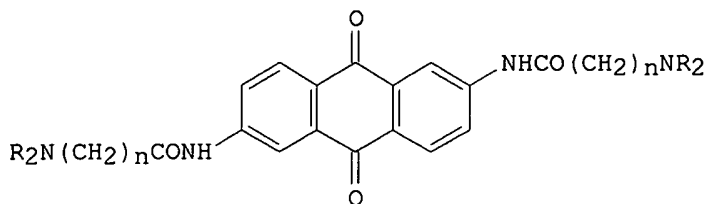


2 REFERENCES IN FILE CA (1957 TO DATE)
2 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 116:193862 CA
TI Anthracene-9,10-diones as potential anticancer agents. Synthesis, DNA-binding, and biological studies on a series of 2,6-disubstituted derivatives
AU Agbandje, Mavis; Jenkins, Terence C.; McKenna, Robert; Reszka, Anthony P.; Neidle, Stephen

CS Cancer Res. Campaign Biomol. Struct. Unit, Inst. Cancer Res.,
Sutton/Surrey, SM2 5NG, UK
SO Journal of Medicinal Chemistry (1992), 35(8), 1418-29
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
GI



AB A series of 2,6-bis(.omega.-aminoalkanamido)anthracene-9,10-diones I (R = Et, CH₂CH₂OH; NR₂ = piperidino, morpholino, piperazino, substituted piperidino, piperazino; n = 1, 2) were prepd. by treatment of the bis(.omega.-haloalkanamides) with secondary amines. The DNA-binding properties of I were evaluated by thermal denaturation studies, unwinding of closed-circular DNA, detn. of assocn. consts. in soln., and examd. by mol. modeling. I (NR₂ = piperidino; n = 1) was examd. by x-ray crystallog. In vitro cytotoxicity data is reported and some indications of structure-activity relationships have been discerned. In particular I (n = 2) have superior activity and, in general, enhanced DNA binding characteristic. It is postulated that the mode of reversible binding of these compds. to DNA involves the side-chains occupying both major and minor grooves and, further, that this may confer cytotoxic properties which are distinct from those of previously reported anthracene-9,10-dione cytotoxins.

REFERENCE 2

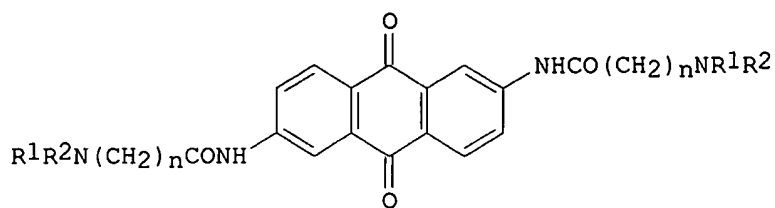
AN 115:49153 CA
TI Preparation of 2,6-bis(aminoalkanoylamino)anthracene-9,10-diones as intercalating agents
IN Neidle, Stephen; Jenkins, Terence Charles; Agbandje, Mavis
PA Cancer Research Technology Ltd., UK
SO PCT Int. Appl., 52 pp.
CODEN: PIXXD2

DT Patent
LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9100265	A1	19910110	WO 1990-GB1004	19900629
	W: JP, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, IT, LU, NL, SE				
	EP 482119	A1	19920429	EP 1990-917804	19900629
	R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, LU, NL, SE				
PRAI	GB 1989-15028		19890630		
	WO 1990-GB1004		19900629		

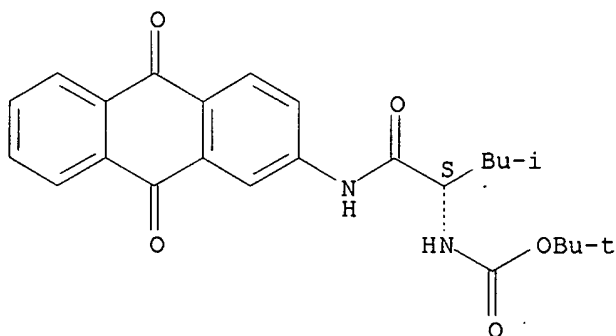
GI



AB The title compds. [I; n = 1, 2, 3; R1, R2 = Et, CH2CH2OH, CH2OH; or R1R2N = piperidino, 2- or 4-(2-hydroxyethyl)piperidino, 2-(hydroxymethyl)piperidino, 4-(2-hydroxyethyl)- or 4-methylpiperidino, morpholino], useful for treating a host suffering from cancer, are prepd. I intercalating into DNA with one side-chain of the mol. residing in each DNA groove, are cytotoxic and non-mutagenic. Thus, a suspension of 14.3 mmol 2,6-bis(3-chloropropionamido)anthracene-9,10-dione in EtOH was gently refluxed and 0.12 mol 4-(2-hydroxyethyl)piperidine in EtOH was added dropwise during 30 min and refluxing was continued for 5 h to give I [n = 2, R1R2N = 4-(2-hydroxyethyl)piperidino] (II). I stabilized various DNA's towards thermal denaturation, the effect of increasing the melting temp. for the DNA by I (n = 2) was comparable to that of mitoxantrone (III) (a known intercalator), and unwinded covalently-colored supercoiled plasmid PM2 DNA. I in vitro showed IC50 of 0.25 - >100 .mu.mol/dm3 against L1210 leukemia cell lines, vs. 0.002 .mu.mol/dm3 with III. II.2AcOH at 200 mg/kg/day i.p. on days 3, 5, 6, and 7 increased 136.8% the life span of mice bearing L1210 leukemia tumor.

L4 ANSWER 25 OF 47 REGISTRY COPYRIGHT 2003 ACS
 RN 114684-56-9 REGISTRY
 CN Carbamic acid, [1-[[[(9,10-dihydro-9,10-dioxo-2-anthracenyl)amino]carbonyl]-3-methylbutyl]-, 1,1-dimethylethyl ester, (S)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C25 H28 N2 O5
 SR CA
 LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
 (*File contains numerically searchable property data)

Absolute stereochemistry.



102

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

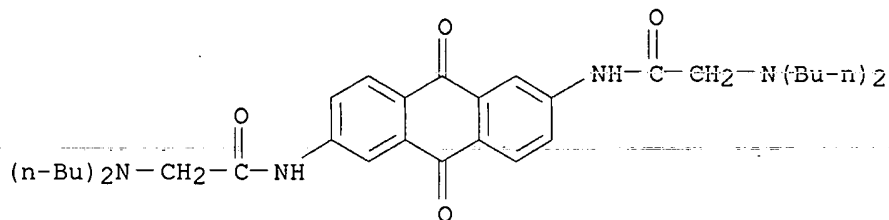
1 REFERENCES IN FILE CA (1957 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 109:6937 CA
 TI New methods and reagents in organic synthesis. 69. A new synthesis of .alpha.-amino acid and peptide amides of aromatic amines using a modified Curtius reaction with diphenyl phosphorazidate
 AU Shioiri, Takayuki; Murata, Mitsuo; Hamada, Yasumasa

CS Fac. Pharm. Sci., Nagoya City Univ., Nagoya, 467, Japan
 SO Chemical & Pharmaceutical Bulletin (1987), 35(7), 2698-704
 CODEN: CPBTAL; ISSN: 0009-2363
 DT Journal
 LA English
 AB Boc-Leu-NHC6H4NO2-p (Boc = Me3CO2C) was prepd. by the reaction of Boc-Leu-OH with the product formed from p-O2NC6H4CO2H through a modified Curtius reaction with di-Ph phosphorazidate. This method is a general method for the synthesis of .alpha.-amino acid arom. amides. This method was applied to the synthesis of peptidase substrate Bz-Ile-Glu(OMe)-Gly-Arg-NHC6H4NO2-p.

L4 ANSWER 26 OF 47 REGISTRY COPYRIGHT 2003 ACS
 RN 108428-65-5 REGISTRY
 CN Acetamide, N,N'-(9,10-dihydro-9,10-dioxo-2,6-anthracenediyl)bis[2-(dibutylamino)- (9CI) (CA INDEX NAME)
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 SR CA
 LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
 (*File contains numerically searchable property data)

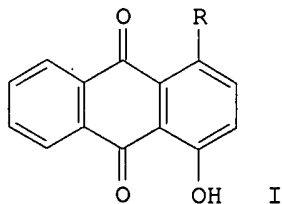


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1 REFERENCES IN FILE CA (1957 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

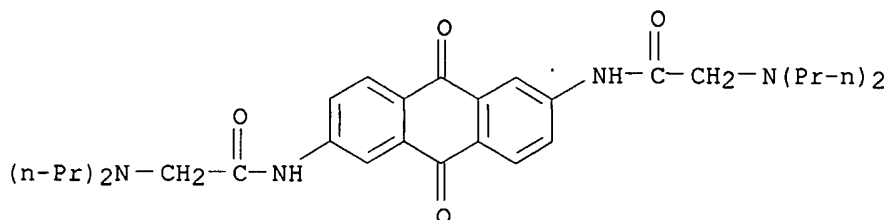
REFERENCE 1

AN 106:213557 CA
 TI Mono- and bis-basic anthraquinones
 AU Hoffmann, Siegfried; Skoelziger, Regina; Witkowski, Werner
 CS Sekt. Chem., Martin-Luther-Univ. Halle-Wittenberg, Halle/Saale, DDR-4020, Ger. Dem. Rep.
 SO Zeitschrift fuer Chemie (1986), 26(6), 206-7
 CODEN: ZECEAL; ISSN: 0044-2402
 DT Journal
 LA German
 GI



AB Aminohydroxyanthracenedione I (R = NH2) in PhNO2 was acylated with ClCH2COCl to give 89% I (R = ClCH2CONH), which was treated with R12NH (R1 = Et, Pr, Bu) to give 29-43% I (R = R12NCH2CONH). 1,5- And 2,6-diamino-9,10-anthracenediones were similarly prepd.

L4 ANSWER 27 OF 47 REGISTRY COPYRIGHT 2003 ACS
 RN 108428-64-4 REGISTRY
 CN Acetamide, N,N'-(9,10-dihydro-9,10-dioxo-2,6-anthracenediyl)bis[2-(dipropylamino)- (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C30 H40 N4 O4
 CI COM
 SR CA
 LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
 (*File contains numerically searchable property data)

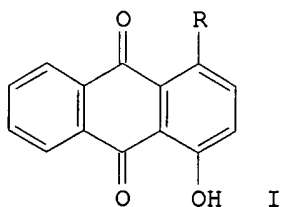


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

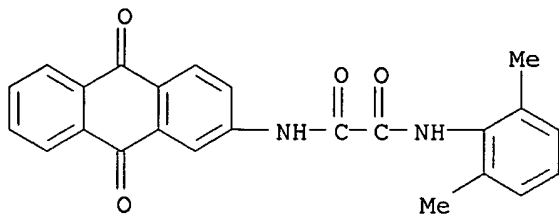
REFERENCE 1

AN 106:213557 CA
 TI Mono- and bis-basic anthraquinones
 AU Hoffmann, Siegfried; Skoelziger, Regina; Witkowski, Werner
 CS Sekt. Chem., Martin-Luther-Univ. Halle-Wittenberg, Halle/Saale, DDR-4020, Ger. Dem. Rep.
 SO Zeitschrift fuer Chemie (1986), 26(6), 206-7
 CODEN: ZECEAL; ISSN: 0044-2402
 DT Journal
 LA German
 GI



AB Aminohydroxyanthracenedione I (R = NH₂) in PhNO₂ was acylated with ClCH₂COCl to give 89% I (R = ClCH₂CONH), which was treated with R₁NH (R₁ = Et, Pr, Bu) to give 29-43% I (R = R₁NCH₂CONH). 1,5- And 2,6-diamino-9,10-anthracenediones were similarly prepd.

L4 ANSWER 28 OF 47 REGISTRY COPYRIGHT 2003 ACS
 RN 100851-12-5 REGISTRY
 CN Ethanediarnide, N-(9,10-dihydro-9,10-dioxo-2-anthracenyl)-N'-(2,6-dimethylphenyl)- (9CI) (CA INDEX NAME)
 MF C24 H18 N2 O4
 SR CA
 LC STN Files: CA, CAPLUS, CASREACT



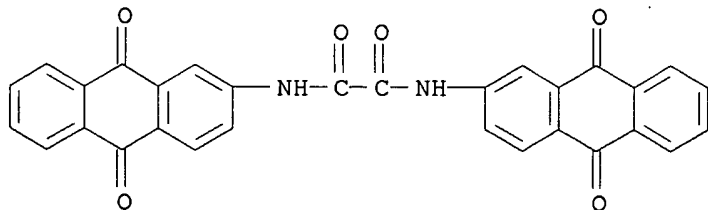
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 104:109164 CA
TI Reaction of amino derivatives of 9,10-anthraquinone with oxalyl chloride
AU Loskutov, V. A.; Savel'ev, V. A.; Konstantinova, A. V.
CS Novosib. Inst. Org. Khim., Novosibirsk, USSR
SO Izvestiya Sibirskogo Otdeleniya Akademii Nauk SSSR, Seriya Khimicheskikh
Nauk (1985), (3), 114-18
CODEN: IZSKAB; ISSN: 0002-3426
DT Journal
LA Russian
AB Title reaction of 1- and 2-amino- and 1-amino-2-chloro-9,10-anthraquinone
gave the corresponding N-anthraquinonyloxamoyl chlorides (I) in 64-95%
yield. Heating RNHCOCOC1 (R = 1- and 2-anthraquinonyl) at 180-190.degree.
and o-Cl2C6H4 gave the N,N'-bis(anthraquinonyl)oxamides in 28-35% yield.
Refluxing I with alcs. and amines or NH3 gave the corresponding oxamidate
esters and oxamides, resp.

L4 ANSWER 29 OF 47 REGISTRY COPYRIGHT 2003 ACS
RN 100851-06-7 REGISTRY
CN Ethanediame, N,N'-bis(9,10-dihydro-9,10-dioxo-2-anthracenyl)- (9CI) (CA
INDEX NAME)
FS 3D CONCORD
MF C30 H16 N2 O6
SR CA
LC STN Files: CA, CAPLUS, CASREACT



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

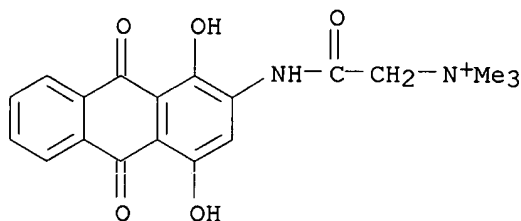
AN 104:109164 CA
TI Reaction of amino derivatives of 9,10-anthraquinone with oxalyl chloride
AU Loskutov, V. A.; Savel'ev, V. A.; Konstantinova, A. V.
CS Novosib. Inst. Org. Khim., Novosibirsk, USSR
SO Izvestiya Sibirskogo Otdeleniya Akademii Nauk SSSR, Seriya Khimicheskikh

Nauk (1985), (3), 114-18
CODEN: IZSKAB; ISSN: 0002-3426

DT Journal
LA Russian

AB Title reaction of 1- and 2-amino- and 1-amino-2-chloro-9,10-anthraquinone gave the corresponding N-anthraquinonyloxamoyl chlorides (I) in 64-95% yield. Heating RNHCOCOC1 ($\text{R} = 1\text{- and } 2\text{-anthraquinonyl}$) at 180-190.degree. and $\text{o-Cl}_2\text{C}_6\text{H}_4$ gave the N,N'-bis(anthraquinonyl)oxamides in 28-35% yield. Refluxing I with alcs. and amines or NH_3 gave the corresponding oxamidate esters and oxamides, resp.

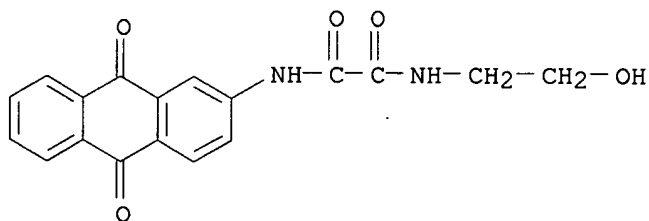
L4 ANSWER 30 OF 47 REGISTRY COPYRIGHT 2003 ACS
RN 98978-74-6 REGISTRY
CN $[[(1,4\text{-Dihydroxy-2-anthraquinonyl})\text{carbamoyl}]\text{methyl}]\text{trimethylammonium chloride (7CI) (CA INDEX NAME)}$
MF $\text{C}_{19}\text{H}_{19}\text{N}_2\text{O}_5 \cdot \text{Cl}$
SR CAOLD
LC STN Files: CAOLD



● Cl^-

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L4 ANSWER 31 OF 47 REGISTRY COPYRIGHT 2003 ACS
RN 92573-44-9 REGISTRY
CN Ethanediamide, N-(9,10-dihydro-9,10-dioxo-2-anthracenyl)-N'-(2-hydroxyethyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF $\text{C}_{18}\text{H}_{14}\text{N}_2\text{O}_5$
LC STN Files: CA, CAPLUS, RTECS*, TOXCENTER
(*File contains numerically searchable property data)



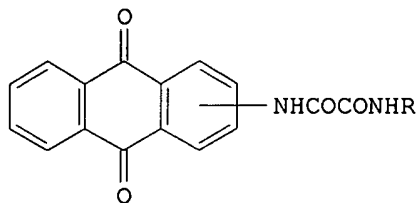
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1957 TO DATE)
4 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 104:101953 CA
TI Synthesis, physicochemical properties and biological activity of substituted amides of anthraquinoneoxamic acids

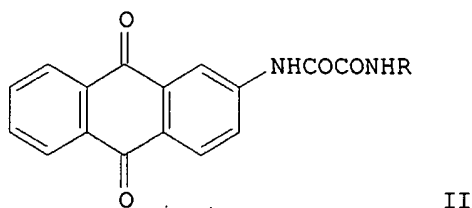
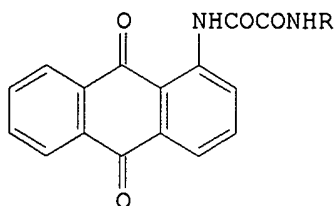
AU Bezuglyi, P. A.; Shtefan, L. M.; Zhuravlev, N. S.; Golubenko, Yu. A.;
 Filippova, L. I.; Drogovoz, S. M.
 CS Kharkov Pharm. Inst., Kharkov, USSR
 SO Farmatsevtichnii Zhurnal (Kiev) (1985), (6), 38-41
 CODEN: FRZKAP; ISSN: 0367-3057
 DT Journal
 LA Ukrainian
 GI



AB Eleven 1- and 2-substituted title compds. [I; R = Me, iso-Pr, (CH₂)₂OH, Me(CH₂)₃, cyclohexyl, PhCH₂, etc.) were prepd. by amidation of 1- and 2-anthraquinoneoxamic acid esters with fatty and fatty-arom. amines. Many I possessed choleretic activity in rats, but with increase in the length of the side chain from C₅ to C₇ choleretic activity was lost completely. Acute i.p. toxicities in mice were low, LD₅₀ values being .gtoreq.5 g/kg.

REFERENCE 2

AN 102:23909 CA
 TI Polarographic study of 9,10-anthraquinone-1- and 2-oxamic acid amides in dimethylformamide
 AU Shapovalov, V. A.
 CS Farm. Inst., Kharkov, USSR
 SO Zhurnal Obshchei Khimii (1984), 54(7), 1637-40
 CODEN: ZOKHA4; ISSN: 0044-460X
 DT Journal
 LA Russian
 GI

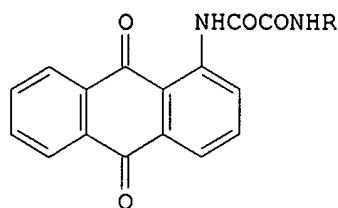


AB The half-wave potentials (E) of the 1st 2 polarog. waves of title compds. I (R = H, Me, CHMe₂, Bu, isopentyl, C₆H₁₁, CH₂Ph) and II (R = H, Me, CHMe₂, Bu, C₆H₁₁, CH₂Ph, CH₂CH₂OH) did not depend on R and corresponded to redn. of the quinone moiety. The E values of I were less neg. than those of II for the 1st 2 waves because of intramol. H bonding in I. Linear Taft plot (.rho. = 0.16) were obtained for the E values of the 3rd waves of I and II; these waves corresponded to redn. of the side chain.

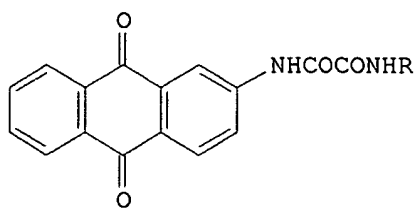
REFERENCE 3

AN 101:210288 CA
 TI Cathodic reduction of 9,10-anthraquinone-1- and 2-oxamic acid amides in the presence of a proton donor
 AU Shapovalov, V. A.
 CS Khar'k. Farm. Inst., Kharkov, USSR
 SO Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1984), 50(7), 729-34

DT Journal
LA Russian
GI



I

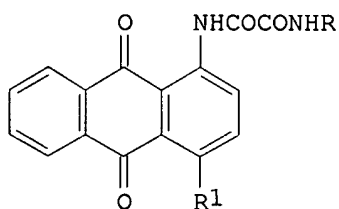


II

AB Polarog. half-wave potentials were detd. for the title compds. (I, II; R = H, Me, CHMe₂, Bu, CH₂CH₂CHMe₂, C₆H₁₁, CH₂Ph, CH₂CH₂OH) in the presence of varying concns. of PhOH. In the absence of PhOH, I and II are reduced first to the semiquinone and then to the quinone dianion (III); finally, the side-chain dicarbonyl moiety is reduced. In the presence of PhOH, III becomes protonated and its further redn. is facilitated and is more complete. The protophilicity (pK) of the semiquinones from I and II were detd. as -3.6 \pm 0.2 and -4.6 \pm 0.2, resp. The difference was linked to intramol. H bonding in the semiquinones from I.

REFERENCE 4

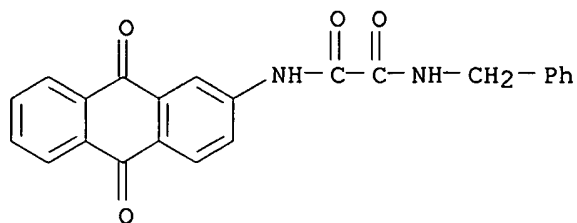
AN 101:170426 CA
TI Electrochemical reduction of oxamic acid amides of the anthraquinone series in an aprotic medium
AU Shapovalov, V. A.; Bezuglyi, P. A.; Shtefan, L. M.; Zhuravlev, N. S.
CS Khar'k. Farm. Inst., Kharkov, USSR
SO Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1984), 50(5), 512-14
CODEN: UKZHAU; ISSN: 0041-6045
DT Journal
LA Russian
GI



I

AB Polarog. data were obtained for the title compds. I (R = H, Me, CHMe₂, Bu, CH₂CHMe₂, C₆H₁₁, CH₂Ph, CH₂CH₂OH; R₁ = H, OH) and the 2-substituted analogs of I (same R; R₁ = H) in DMF, and linear correlations were obtained between the half-wave potentials and σ^* consts. The quinone moiety of I is reduced first in a stepwise 2-electron process; at more neg. potentials the dicarbonyl moiety in the side chain is reduced.

L4 ANSWER 32 OF 47 REGISTRY COPYRIGHT 2003 ACS
RN 92573-43-8 REGISTRY
CN Ethanediarnide, N-(9,10-dihydro-9,10-dioxo-2-anthracenyl)-N'-(phenylmethyl)-
(9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C23 H16 N2 O4
LC STN Files: CA, CAPLUS, RTECS*, TOXCENTER
(*File contains numerically searchable property data)

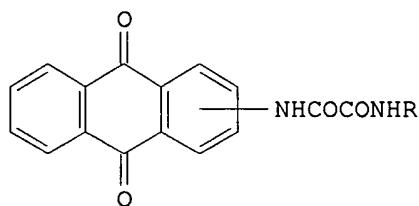


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1957 TO DATE)
4 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

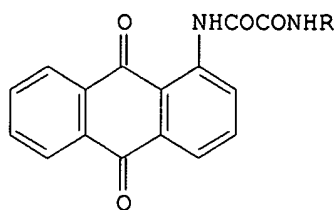
AN 104:101953 CA
TI Synthesis, physicochemical properties and biological activity of substituted amides of anthraquinoneoxamic acids
AU Bezuglyi, P. A.; Shtefan, L. M.; Zhuravlev, N. S.; Golubenko, Yu. A.; Filippova, L. I.; Drogovoz, S. M.
CS Kharkov Pharm. Inst., Kharkov, USSR
SO Farmatsevtichnii Zhurnal (Kiev) (1985), (6), 38-41
CODEN: FRZKAP; ISSN: 0367-3057
DT Journal
LA Ukrainian
GI



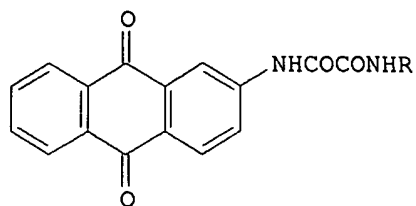
AB Eleven 1- and 2-substituted title compds. [I; R = Me, iso-Pr, (CH₂)₂OH, Me(CH₂)₃, cyclohexyl, PhCH₂, etc.) were prepd. by amidation of 1- and 2-anthraquinoneoxamic acid esters with fatty and fatty-arom. amines. Many I possessed choleretic activity in rats, but with increase in the length of the side chain from C₅ to C₇ choleretic activity was lost completely. Acute i.p. toxicities in mice were low, LD₅₀ values being .gtoreq.5 g/kg.

REFERENCE 2

AN 102:23909 CA
TI Polarographic study of 9,10-anthraquinone-1- and 2-oxamic acid amides in dimethylformamide
AU Shapovalov, V. A.
CS Farm. Inst., Kharkov, USSR
SO Zhurnal Obshchei Khimii (1984), 54(7), 1637-40
CODEN: ZOKHA4; ISSN: 0044-460X
DT Journal
LA Russian
GI



I

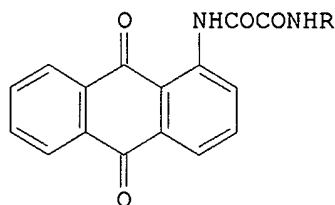


II

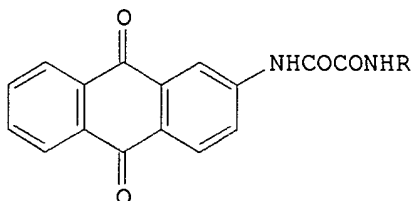
AB The half-wave potentials (E) of the 1st 2 polarog. waves of title compds. I (R = H, Me, CHMe₂, Bu, isopentyl, C₆H₁₁, CH₂Ph) and II (R = H, Me, CHMe₂, Bu, C₆H₁₁, CH₂Ph, CH₂CH₂OH) did not depend on R and corresponded to redn. of the quinone moiety. The E values of I were less neg. than those of II for the 1st 2 waves because of intramol. H bonding in I. Linear Taft plot (.rho. = 0.16) were obtained for the E values of the 3rd waves of I and II; these waves corresponded to redn. of the side chain.

REFERENCE 3

AN 101:210288 CA
 TI Cathodic reduction of 9,10-anthraquinone-1- and 2-oxamic acid amides in the presence of a proton donor
 AU Shapovalov, V. A.
 CS Khar'k. Farm. Inst., Kharkov, USSR
 SO Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1984), 50(7), 729-34
 CODEN: UKZHAU; ISSN: 0041-6045
 DT Journal
 LA Russian
 GI



I

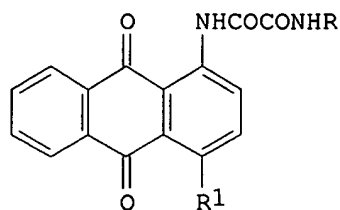


II

AB Polarog. half-wave potentials were detd. for the title compds. (I, II; R = H, Me, CHMe₂, Bu, CH₂CH₂CHMe₂, C₆H₁₁, CH₂Ph, CH₂CH₂OH) in the presence of varying concns. of PhOH. In the absence of PhOH, I and II are reduced first to the semiquinone and then to the quinone dianion (III); finally, the side-chain dicarbonyl moiety is reduced. In the presence of PhOH, III becomes protonated and its further redn. is facilitated and is more complete. The protophilicity (pK) of the semiquinones from I and II were detd. as -3.6 +/- 0.2 and -4.6 +/- 0.2, resp. The difference was linked to intramol. H bonding in the semiquinones from I.

REFERENCE 4

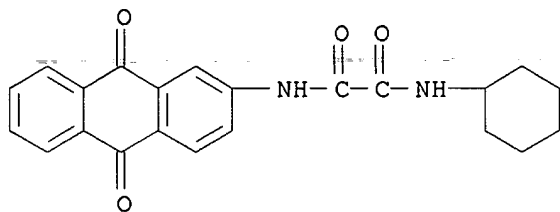
AN 101:170426 CA
 TI Electrochemical reduction of oxamic acid amides of the anthraquinone series in an aprotic medium
 AU Shapovalov, V. A.; Bezuglyi, P. A.; Shtefan, L. M.; Zhuravlev, N. S.
 CS Khar'k. Farm. Inst., Kharkov, USSR
 SO Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1984), 50(5), 512-14
 CODEN: UKZHAU; ISSN: 0041-6045
 DT Journal
 LA Russian
 GI



I

AB Polarog. data were obtained for the title compds. I (R = H, Me, CHMe₂, Bu, CH₂CHMe₂, C₆H₁₁, CH₂Ph, CH₂CH₂OH; R₁ = H, OH) and the 2-substituted analogs of I (same R; R₁ = H) in DMF, and linear correlations were obtained between the half-wave potentials and σ consts. The quinone moiety of I is reduced first in a stepwise 2-electron process; at more neg. potentials the dicarbonyl moiety in the side chain is reduced.

L4 ANSWER 33 OF 47 REGISTRY COPYRIGHT 2003 ACS
 RN 92573-42-7 REGISTRY
 CN Ethanediame, N-cyclohexyl-N'-(9,10-dihydro-9,10-dioxo-2-anthracenyl)-
 (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C22 H20 N2 O4
 LC STN Files: CA, CAPLUS

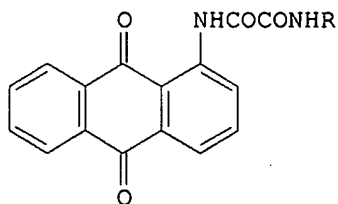


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

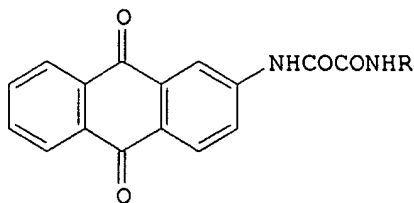
3 REFERENCES IN FILE CA (1957 TO DATE)
 3 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 102:23909 CA
 TI Polarographic study of 9,10-anthraquinone-1- and 2-oxamic acid amides in dimethylformamide
 AU Shapovalov, V. A.
 CS Farm. Inst., Kharkov, USSR
 SO Zhurnal Obshchei Khimii (1984), 54(7), 1637-40
 CODEN: ZOKHA4; ISSN: 0044-460X
 DT Journal
 LA Russian
 GI



I



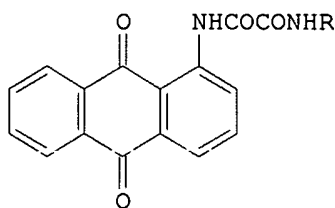
II

AB The half-wave potentials (E) of the 1st 2 polarog. waves of title compds.

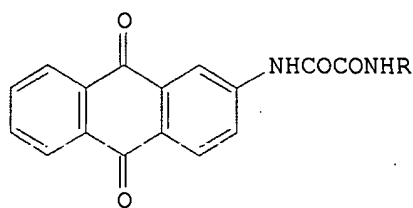
I (R = H, Me, CHMe₂, Bu, isopentyl, C₆H₁₁, CH₂Ph) and II (R = H, Me, CHMe₂, Bu, C₆H₁₁, CH₂Ph, CH₂CH₂OH) did not depend on R and corresponded to redn. of the quinone moiety. The E values of I were less neg. than those of II for the 1st 2 waves because of intramol. H bonding in I. Linear Taft plot ($\rho = 0.16$) were obtained for the E values of the 3rd waves of I and II; these waves corresponded to redn. of the side chain.

REFERENCE 2

AN 101:210288 CA
 TI Cathodic reduction of 9,10-anthraquinone-1- and 2-oxamic acid amides in the presence of a proton donor
 AU Shapovalov, V. A.
 CS Khar'k. Farm. Inst., Kharkov, USSR
 SO Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1984), 50(7), 729-34
 CODEN: UKZHAU; ISSN: 0041-6045
 DT Journal
 LA Russian
 GI



I

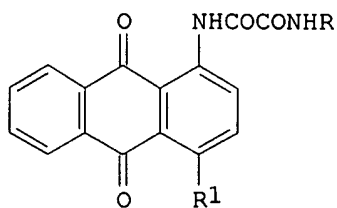


II

AB Polarog. half-wave potentials were detd. for the title compds. (I, II; R = H, Me, CHMe₂, Bu, CH₂CH₂CHMe₂, C₆H₁₁, CH₂Ph, CH₂CH₂OH) in the presence of varying concns. of PhOH. In the absence of PhOH, I and II are reduced first to the semiquinone and then to the quinone dianion (III); finally, the side-chain dicarbonyl moiety is reduced. In the presence of PhOH, III becomes protonated and its further redn. is facilitated and is more complete. The protophilicity (pK) of the semiquinones from I and II were detd. as -3.6 \pm 0.2 and -4.6 \pm 0.2, resp. The difference was linked to intramol. H bonding in the semiquinones from I.

REFERENCE 3

AN 101:170426 CA
 TI Electrochemical reduction of oxamic acid amides of the anthraquinone series in an aprotic medium
 AU Shapovalov, V. A.; Bezuglyi, P. A.; Shtefan, L. M.; Zhuravlev, N. S.
 CS Khar'k. Farm. Inst., Kharkov, USSR
 SO Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1984), 50(5), 512-14
 CODEN: UKZHAU; ISSN: 0041-6045
 DT Journal
 LA Russian
 GI

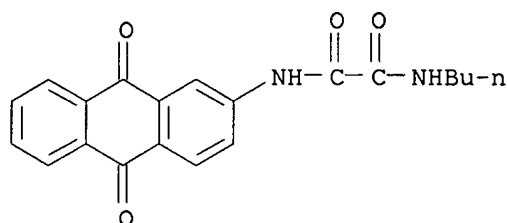


I

AB Polarog. data were obtained for the title compds. I (R = H, Me, CHMe₂, Bu, CH₂CHMe₂, C₆H₁₁, CH₂Ph, CH₂CH₂OH; R₁ = H, OH) and the 2-substituted

analogs of I (same R; R1 = H) in DMF, and linear correlations were obtained between the half-wave potentials and σ consts. The quinone moiety of I is reduced first in a stepwise 2-electron process; at more neg. potentials the dicarbonyl moiety in the side chain is reduced.

L4 ANSWER 34 OF 47 REGISTRY COPYRIGHT 2003 ACS
 RN 92573-41-6 REGISTRY
 CN Ethanediamide, N-butyl-N'-(9,10-dihydro-9,10-dioxo-2-anthracenyl)- (9CI)
 (CA INDEX NAME)
 FS 3D CONCORD
 MF C20 H18 N2 O4
 LC STN Files: CA, CAPLUS

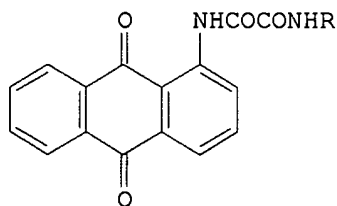


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

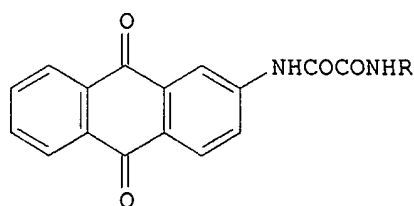
3 REFERENCES IN FILE CA (1957 TO DATE)
 3 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 102:23909 CA
 TI Polarographic study of 9,10-anthraquinone-1- and 2-oxamic acid amides in dimethylformamide
 AU Shapovalov, V. A.
 CS Farm. Inst., Kharkov, USSR
 SO Zhurnal Obshchei Khimii (1984), 54(7), 1637-40
 CODEN: ZOKHA4; ISSN: 0044-460X
 DT Journal
 LA Russian
 GI



I



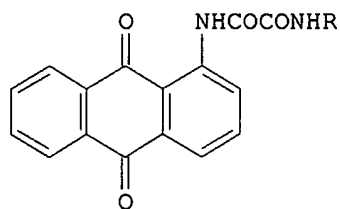
II

AB The half-wave potentials (E) of the 1st 2 polarog. waves of title compds. I (R = H, Me, CHMe2, Bu, isopentyl, C6H11, CH2Ph) and II (R = H, Me, CHMe2, Bu, C6H11, CH2Ph, CH2CH2OH) did not depend on R and corresponded to redn. of the quinone moiety. The E values of I were less neg. than those of II for the 1st 2 waves because of intramol. H bonding in I. Linear Taft plot (ρ = 0.16) were obtained for the E values of the 3rd waves of I and II; these waves corresponded to redn. of the side chain.

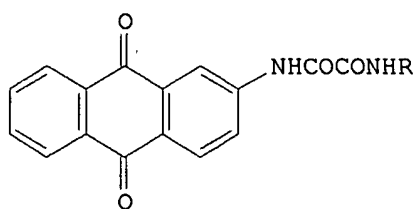
REFERENCE 2

AN 101:210288 CA
 TI Cathodic reduction of 9,10-anthraquinone-1- and 2-oxamic acid amides in the presence of a proton donor

AU Shapovalov, V. A.
 CS Khar'k. Farm. Inst., Kharkov, USSR
 SO Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1984), 50(7), 729-34
 CODEN: UKZHAU; ISSN: 0041-6045
 DT Journal
 LA Russian
 GI



I

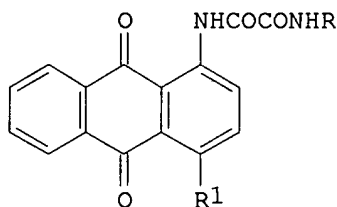


II

AB Polarog. half-wave potentials were detd. for the title compds. (I, II; R = H, Me, CHMe₂, Bu, CH₂CH₂CHMe₂, C₆H₁₁, CH₂Ph, CH₂CH₂OH) in the presence of varying concns. of PhOH. In the absence of PhOH, I and II are reduced first to the semiquinone and then to the quinone dianion (III); finally, the side-chain dicarbonyl moiety is reduced. In the presence of PhOH, III becomes protonated and its further redn. is facilitated and is more complete. The protophilicity (pK) of the semiquinones from I and II were detd. as -3.6 ± 0.2 and -4.6 ± 0.2, resp. The difference was linked to intramol. H bonding in the semiquinones from I.

REFERENCE 3

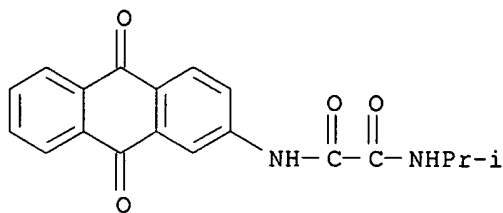
AN 101:170426 CA
 TI Electrochemical reduction of oxamic acid amides of the anthraquinone series in an aprotic medium
 AU Shapovalov, V. A.; Bezuglyi, P. A.; Shtefan, L. M.; Zhuravlev, N. S.
 CS Khar'k. Farm. Inst., Kharkov, USSR
 SO Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1984), 50(5), 512-14
 CODEN: UKZHAU; ISSN: 0041-6045
 DT Journal
 LA Russian
 GI



I

AB Polarog. data were obtained for the title compds. I (R = H, Me, CHMe₂, Bu, CH₂CHMe₂, C₆H₁₁, CH₂Ph, CH₂CH₂OH; R₁ = H, OH) and the 2-substituted analogs of I (same R; R₁ = H) in DMF, and linear correlations were obtained between the half-wave potentials and σ^* consts. The quinone moiety of I is reduced first in a stepwise 2-electron process; at more neg. potentials the dicarbonyl moiety in the side chain is reduced.

L4 ANSWER 35 OF 47 REGISTRY COPYRIGHT 2003 ACS
 RN 92573-40-5 REGISTRY
 CN Ethanediame, N-(9,10-dihydro-9,10-dioxo-2-anthracenyl)-N'-(1-methylethyl)- (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C19 H16 N2 O4
 LC STN Files: CA, CAPLUS, RTECS*, TOXCENTER

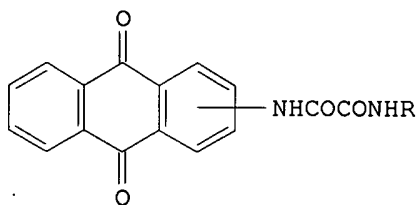


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1957 TO DATE)
4 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 104:101953 CA
TI Synthesis, physicochemical properties and biological activity of substituted amides of anthraquinoneoxamic acids
AU Bezuglyi, P. A.; Shtefan, L. M.; Zhuravlev, N. S.; Golubenko, Yu. A.; Filippova, L. I.; Drogovoz, S. M.
CS Kharkov Pharm. Inst., Kharkov, USSR
SO Farmatsevtichnii Zhurnal (Kiev) (1985), (6), 38-41
CODEN: FRZKAP; ISSN: 0367-3057
DT Journal
LA Ukranian
GI

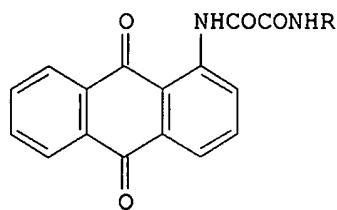


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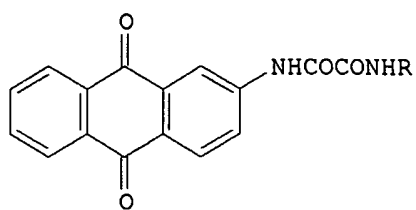
AB Eleven 1- and 2-substituted title compds. [I; R = Me, iso-Pr, (CH₂)₂OH, Me(CH₂)₃, cyclohexyl, PhCH₂, etc.) were prepd. by amidation of 1- and 2-anthraquinoneoxamic acid esters with fatty and fatty-arom. amines. Many I possessed choleretic activity in rats, but with increase in the length of the side chain from C₅ to C₇ choleretic activity was lost completely. Acute i.p. toxicities in mice were low, LD₅₀ values being .gtoreq.5 g/kg.

REFERENCE 2

AN 102:23909 CA
TI Polarographic study of 9,10-anthraquinone-1- and 2-oxamic acid amides in dimethylformamide
AU Shapovalov, V. A.
CS Farm. Inst., Kharkov, USSR
SO Zhurnal Obshchei Khimii (1984), 54(7), 1637-40
CODEN: ZOKHA4; ISSN: 0044-460X
DT Journal
LA Russian
GI



I

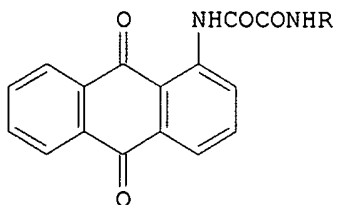


II

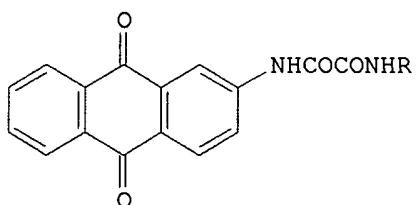
AB The half-wave potentials (E) of the 1st 2 polarog. waves of title compds. I (R = H, Me, CHMe₂, Bu, isopentyl, C₆H₁₁, CH₂Ph) and II (R = H, Me, CHMe₂, Bu, C₆H₁₁, CH₂Ph, CH₂CH₂OH) did not depend on R and corresponded to redn. of the quinone moiety. The E values of I were less neg. than those of II for the 1st 2 waves because of intramol. H bonding in I. Linear Taft plot ($\rho = 0.16$) were obtained for the E values of the 3rd waves of I and II; these waves corresponded to redn. of the side chain.

REFERENCE 3

AN 101:210288 CA
 TI Cathodic reduction of 9,10-anthraquinone-1- and 2-oxamic acid amides in the presence of a proton donor
 AU Shapovalov, V. A.
 CS Khar'k. Farm. Inst., Kharkov, USSR
 SO Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1984), 50(7), 729-34
 CODEN: UKZHAU; ISSN: 0041-6045
 DT Journal
 LA Russian
 GI



I

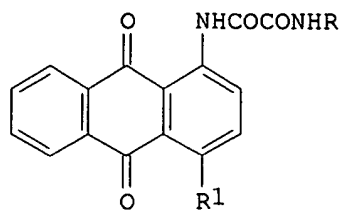


II

AB Polarog. half-wave potentials were detd. for the title compds. (I, II; R = H, Me, CHMe₂, Bu, CH₂CH₂CHMe₂, C₆H₁₁, CH₂Ph, CH₂CH₂OH) in the presence of varying concns. of PhOH. In the absence of PhOH, I and II are reduced first to the semiquinone and then to the quinone dianion (III); finally, the side-chain dicarbonyl moiety is reduced. In the presence of PhOH, III becomes protonated and its further redn. is facilitated and is more complete. The protophilicity (pK) of the semiquinones from I and II were detd. as -3.6 \pm 0.2 and -4.6 \pm 0.2, resp. The difference was linked to intramol. H bonding in the semiquinones from I.

REFERENCE 4

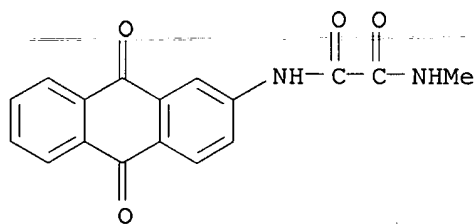
AN 101:170426 CA
 TI Electrochemical reduction of oxamic acid amides of the anthraquinone series in an aprotic medium
 AU Shapovalov, V. A.; Bezuglyi, P. A.; Shtefan, L. M.; Zhuravlev, N. S.
 CS Khar'k. Farm. Inst., Kharkov, USSR
 SO Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1984), 50(5), 512-14
 CODEN: UKZHAU; ISSN: 0041-6045
 DT Journal
 LA Russian
 GI



I

AB Polarog. data were obtained for the title compds. I (R = H, Me, CHMe₂, Bu, CH₂CHMe₂, C₆H₁₁, CH₂Ph, CH₂CH₂OH; R₁ = H, OH) and the 2-substituted analogs of I (same R; R₁ = H) in DMF, and linear correlations were obtained between the half-wave potentials and .sigma.* consts. The quinone moiety of I is reduced first in a stepwise 2-electron process; at more neg. potentials the dicarbonyl moiety in the side chain is reduced.

L4 ANSWER 36 OF 47 REGISTRY COPYRIGHT 2003 ACS
 RN 92573-39-2 REGISTRY
 CN Ethanediame, N-(9,10-dihydro-9,10-dioxo-2-anthracenyl)-N'-methyl- (9CI)
 (CA INDEX NAME)
 FS 3D CONCORD
 MF C17 H12 N2 O4
 LC STN Files: CA, CAPLUS, RTECS*, TOXCENTER
 (*File contains numerically searchable property data)

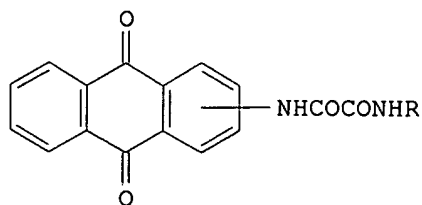


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1957 TO DATE)
 4 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 104:101953 CA
 TI Synthesis, physicochemical properties and biological activity of substituted amides of anthraquinoneoxamic acids
 AU Bezuglyi, P. A.; Shtefan, L. M.; Zhuravlev, N. S.; Golubenko, Yu. A.; Filippova, L. I.; Drogovoz, S. M.
 CS Kharkov Pharm. Inst., Kharkov, USSR
 SO Farmatsevtichnij Zhurnal (Kiev) (1985), (6), 38-41
 CODEN: FRZKAP; ISSN: 0367-3057
 DT Journal
 LA Ukranian
 GI

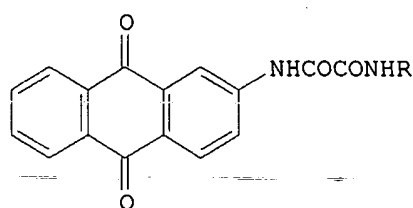
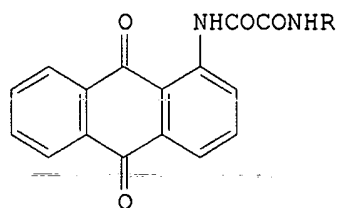


I

AB Eleven 1- and 2-substituted title compds. [I; R = Me, iso-Pr, (CH₂)₂OH, Me(CH₂)₃, cyclohexyl, PhCH₂, etc.) were prepd. by amidation of 1- and 2-anthraquinoneoxamic acid esters with fatty and fatty-arom. amines. Many I possessed choleric activity in rats, but with increase in the length of the side chain from C5 to C7 choleric activity was lost completely. Acute i.p. toxicities in mice were low, LD₅₀ values being .gtoreq.5 g/kg.

REFERENCE 2

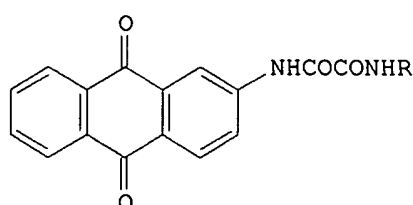
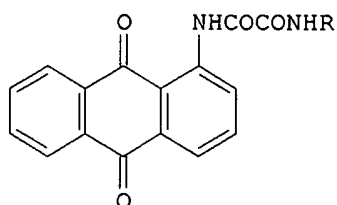
AN 102:23909 CA
 TI Polarographic study of 9,10-anthraquinone-1- and 2-oxamic acid amides in dimethylformamide
 AU Shapovalov, V. A.
 CS Farm. Inst., Kharkov, USSR
 SO Zhurnal Obshchei Khimii (1984), 54(7), 1637-40
 CODEN: ZOKHA4; ISSN: 0044-460X
 DT Journal
 LA Russian
 GI



AB The half-wave potentials (E) of the 1st 2 polarog. waves of title compds. I (R = H, Me, CHMe₂, Bu, isopentyl, C₆H₁₁, CH₂Ph) and II (R = H, Me, CHMe₂, Bu, C₆H₁₁, CH₂Ph, CH₂CH₂OH) did not depend on R and corresponded to redn. of the quinone moiety. The E values of I were less neg. than those of II for the 1st 2 waves because of intramol. H bonding in I. Linear Taft plot (.rho. = 0.16) were obtained for the E values of the 3rd waves of I and II; these waves corresponded to redn. of the side chain.

REFERENCE 3

AN 101:210288 CA
 TI Cathodic reduction of 9,10-anthraquinone-1- and 2-oxamic acid amides in the presence of a proton donor
 AU Shapovalov, V. A.
 CS Khar'k. Farm. Inst., Kharkov, USSR
 SO Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1984), 50(7), 729-34
 CODEN: UKZHAU; ISSN: 0041-6045
 DT Journal
 LA Russian
 GI

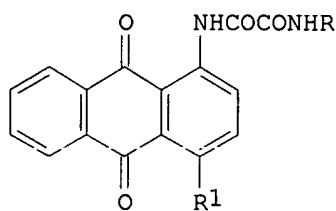


AB Polarog. half-wave potentials were detd. for the title compds. (I, II; R = H, Me, CHMe₂, Bu, CH₂CH₂CHMe₂, C₆H₁₁, CH₂Ph, CH₂CH₂OH) in the presence of varying concns. of PhOH. In the absence of PhOH, I and II are reduced

first to the semiquinone and then to the quinone dianion (III); finally, the side-chain dicarbonyl moiety is reduced. In the presence of PhOH, III becomes protonated and its further redn. is facilitated and is more complete. The protophilicity (pK) of the semiquinones from I and II were detd. as -3.6 ± 0.2 and -4.6 ± 0.2 , resp. The difference was linked to intramol. H bonding in the semiquinones from I.

REFERENCE 4

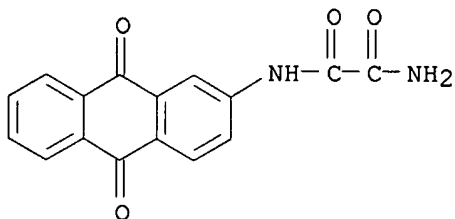
AN 101:170426 CA
 TI Electrochemical reduction of oxamic acid amides of the anthraquinone series in an aprotic medium
 AU Shapovalov, V. A.; Bezuglyi, P. A.; Shtefan, L. M.; Zhuravlev, N. S.
 CS Khar'k. Farm. Inst., Kharkov, USSR
 SO Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1984), 50(5), 512-14
 CODEN: UKZHAU; ISSN: 0041-6045
 DT Journal
 LA Russian
 GI



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AB Polarog. data were obtained for the title compds. I (R = H, Me, CHMe₂, Bu, CH₂CHMe₂, C₆H₁₁, CH₂Ph, CH₂CH₂OH; R₁ = H, OH) and the 2-substituted analogs of I (same R; R₁ = H) in DMF, and linear correlations were obtained between the half-wave potentials and σ consts. The quinone moiety of I is reduced first in a stepwise 2-electron process; at more neg. potentials the dicarbonyl moiety in the side chain is reduced.

L4 ANSWER 37 OF 47 REGISTRY COPYRIGHT 2003 ACS
 RN 92573-38-1 REGISTRY
 CN Ethanediame, (9,10-dihydro-9,10-dioxo-2-anthracenyl)- (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C16 H10 N2 O4
 LC STN Files: CA, CAPLUS



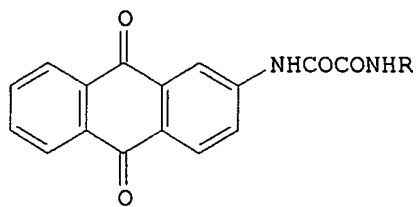
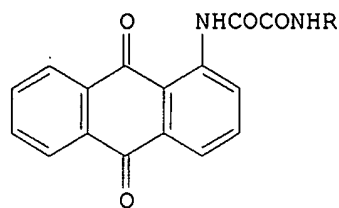
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1957 TO DATE)
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REFERENCE 1

AN 102:23909 CA
 TI Polarographic study of 9,10-anthraquinone-1- and 2-oxamic acid amides in

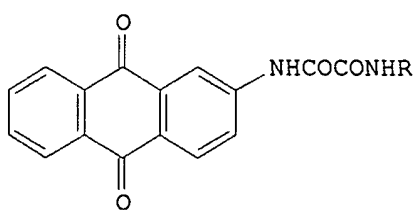
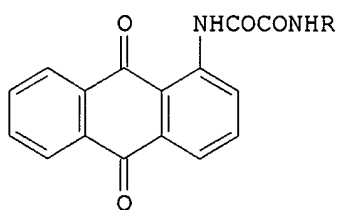
AU dimethylformamide
 CS Shapovalov, V. A.
 SO Farm. Inst., Kharkov, USSR
 Zhurnal Obshchei Khimii (1984), 54(7), 1637-40
 CODEN: ZOKHA4; ISSN: 0044-460X
 DT Journal
 LA Russian
 GI



AB The half-wave potentials (E) of the 1st 2 polarog. waves of title compds. I (R = H, Me, CHMe₂, Bu, isopentyl, C₆H₁₁, CH₂Ph) and II (R = H, Me, CHMe₂, Bu, C₆H₁₁, CH₂Ph, CH₂CH₂OH) did not depend on R and corresponded to redn. of the quinone moiety. The E values of I were less neg. than those of II for the 1st 2 waves because of intramol. H bonding in I. Linear Taft plot (ρ = 0.16) were obtained for the E values of the 3rd waves of I and II; these waves corresponded to redn. of the side chain.

REFERENCE 2

AN 101:210288 CA
 TI Cathodic reduction of 9,10-anthraquinone-1- and 2-oxamic acid amides in the presence of a proton donor
 AU Shapovalov, V. A.
 CS Khar'k. Farm. Inst., Kharkov, USSR
 SO Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1984), 50(7), 729-34
 CODEN: UKZHAU; ISSN: 0041-6045
 DT Journal
 LA Russian
 GI

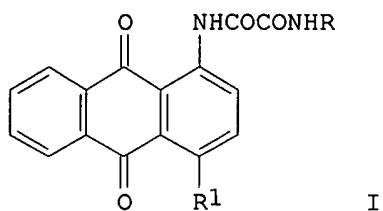


AB Polarog. half-wave potentials were detd. for the title compds. (I, II; R = H, Me, CHMe₂, Bu, CH₂CH₂CHMe₂, C₆H₁₁, CH₂Ph, CH₂CH₂OH) in the presence of varying concns. of PhOH. In the absence of PhOH, I and II are reduced first to the semiquinone and then to the quinone dianion (III); finally, the side-chain dicarbonyl moiety is reduced. In the presence of PhOH, III becomes protonated and its further redn. is facilitated and is more complete. The protophilicity (pK) of the semiquinones from I and II were detd. as -3.6 \pm 0.2 and -4.6 \pm 0.2, resp. The difference was linked to intramol. H bonding in the semiquinones from I.

REFERENCE 3

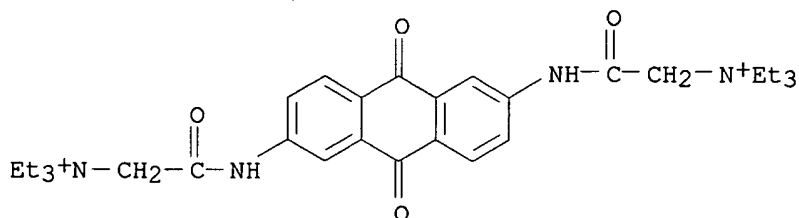
AN 101:170426 CA
 TI Electrochemical reduction of oxamic acid amides of the anthraquinone series in an aprotic medium

AU Shapovalov, V. A.; Bezuglyi, P. A.; Shtefan, L. M.; Zhuravlev, N. S.
 CS Khar'k. Farm. Inst., Kharkov, USSR
 SO Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1984), 50(5), 512-14
 CODEN: UKZHAU; ISSN: 0041-6045
 DT Journal
 LA Russian
 GI



AB Polarog. data were obtained for the title compds. I (R = H, Me, CHMe₂, Bu, CH₂CHMe₂, C₆H₁₁, CH₂Ph, CH₂CH₂OH; R₁ = H, OH) and the 2-substituted analogs of I (same R; R₁ = H) in DMF, and linear correlations were obtained between the half-wave potentials and .sigma.* consts. The quinone moiety of I is reduced first in a stepwise 2-electron process; at more neg. potentials the dicarbonyl moiety in the side chain is reduced.

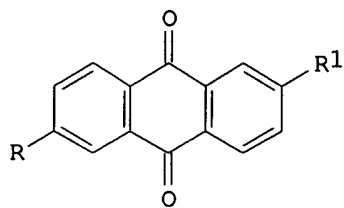
L4 ANSWER 38 OF 47 REGISTRY COPYRIGHT 2003 ACS
 RN 72966-61-1 REGISTRY
 CN Ethanaminium, 2,2'-[(9,10-dihydro-9,10-dioxo-2,6=anthracenediyl)diimino]bis[N,N,N-triethyl-2-oxo-, dichloride (9CI) (CA INDEX NAME)
 MF C30 H42 N4 O4 . 2 Cl
 LC STN Files: CA, CAPLUS



1 REFERENCES IN FILE CA (1957 TO DATE)
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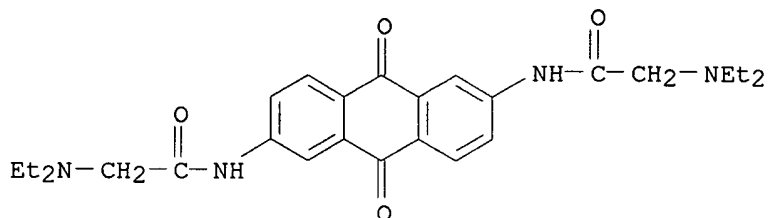
REFERENCE 1

AN 92:110720 CA
 TI Chemotherapeutically active anthraquinones. I. Aminoanthraquinones
 AU Winkelmann, E.; Raether, W.
 CS Hoechst A.-G., Frankfurt/Main, D-6230, Fed. Rep. Ger.
 SO Arzneimittel-Forschung (1979), 29(10), 1504-9
 CODEN: ARZNAD; ISSN: 0004-4172
 DT Journal
 LA English
 GI



AB Anthraquinones I (R = R1 = optionally substituted acylamino and alkyleneamino; R = H, R1 = N:CHNMe₂; R = R1 = aminoalkyleneamino) (46 compds.) were prepd. by substitution of the corresponding amines by chloroacyl chlorides or amidation of the acylamines. I (R = R1 = aminoalkyleneamino) most effectively controlled *Trichomonas vaginalis*, *T. fetus* and *Entameba histolytica*. Thus, anthraquinone systems and bis(amidino) groups are needed for protozoacidal activity.

L4 ANSWER 39 OF 47 REGISTRY COPYRIGHT 2003 ACS
 RN 72966-57-5 REGISTRY
 CN Acetamide, N,N'-(9,10-dihydro-9,10-dioxo-2,6-anthracenediyl)bis[2-(diethylamino)- (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C26 H32 N4 O4
 CI COM
 LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, TOXCENTER
 (*File contains numerically searchable property data)



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7 REFERENCES IN FILE CA (1957 TO DATE)
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REFERENCE 1

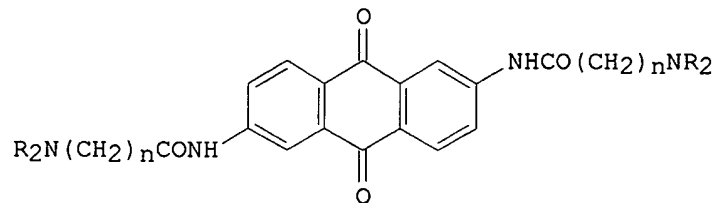
AN 129:239565 CA
 TI Anthracene-9,10-diones as Potential Anticancer Agents: Bacterial Mutation Studies of Amido-Substituted Derivatives Reveal an Unexpected Lack of Mutagenicity
 AU Venitt, Stanley; Crofton-Sleigh, Christopher; Agbandje, Mavis; Jenkins, Terence C.; Neidle, Stephen
 CS Section of Molecular Carcinogenesis and Cancer Research Campaign Biomolecular Structure Unit The Institute of Cancer Research, Royal Cancer Hospital, Sutton, Surrey, SM2 5NG, UK
 SO Journal of Medicinal Chemistry (1998), 41(19), 3748-3752
 CODEN: JMCMAR; ISSN: 0022-2623
 PB American Chemical Society
 DT Journal
 LA English
 AB Fifteen anthracene-9,10-dione ("anthraquinone") derivs. with (.omega.-aminoalkyl)carboxamido substituents at the 1-, 2-, 1,4-, or 2,6-ring positions were tested for bacterial mutagenicity in reverse-mutation assays using *Salmonella typhimurium* frameshift strains TA1538, TA98, and TA97a, in the presence and absence of a metabolic activation system prepd. from the livers of rats treated with Aroclor

1254. Six of the compds. were also tested in *S. typhimurium* TA100 and *Escherichia coli* WP2uvrApKM101 strains, which carry mutations particularly sensitive to reversion by DNA base-pair substitution. Two structurally related compds., mitoxantrone and bisantrene, were tested in parallel as pos. controls. Mitoxantrone was mutagenic to *S. typhimurium* TA1538 and TA98, whereas bisantrene was weakly mutagenic to both these strains but strongly mutagenic toward the TA97a variant. By contrast, although they are also DNA-binding intercalators, none of the amide-functionalized anthracene-9,10-diones of the present study showed significant mutagenic activity in any of the bacterial strains examd. Further, neither substituent position nor systematic alterations in the nature of attached side chains appeared to induce mutagenicity with these agents, although other studies have shown that such structural factors markedly influence their cytotoxic potencies toward mammalian cells in vitro.

RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 2

AN 116:193862 CA
TI Anthracene-9,10-diones as potential anticancer agents. Synthesis, DNA-binding, and biological studies on a series of 2,6-disubstituted derivatives
AU Agbandje, Mavis; Jenkins, Terence C.; McKenna, Robert; Reszka, Anthony P.; Neidle, Stephen
CS Cancer Res. Campaign Biomol. Struct. Unit, Inst. Cancer Res., Sutton/Surrey, SM2 5NG, UK
SO Journal of Medicinal Chemistry (1992), 35(8), 1418-29
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
GI



I

AB A series of 2,6-bis(omega-aminoalkanamido)anthracene-9,10-diones I (R = Et, CH₂CH₂OH; NR₂ = piperidino, morpholino, piperazino, substituted piperidino, piperazino; n = 1, 2) were prepd. by treatment of the bis(omega-haloalkanamides) with secondary amines. The DNA-binding properties of I were evaluated by thermal denaturation studies, unwinding of closed-circular DNA, detn. of assocn. consts. in soln., and examd. by mol. modeling. I (NR₂ = piperidino; n = 1) was examd. by x-ray crystallog. In vitro cytotoxicity data is reported and some indications of structure-activity relationships have been discerned. In particular I (n = 2) have superior activity and, in general, enhanced DNA binding characteristic. It is postulated that the mode of reversible binding of these compds. to DNA involves the side-chains occupying both major and minor grooves and, further, that this may confer cytotoxic properties which are distinct from those of previously reported anthracene-9,10-dione cytotoxins.

REFERENCE 3

AN 115:49153 CA
TI Preparation of 2,6-bis(aminoalkanoylamino)anthracene-9,10-diones as intercalating agents
IN Neidle, Stephen; Jenkins, Terence Charles; Agbandje, Mavis
PA Cancer Research Technology Ltd., UK

SO PCT Int. Appl., 52 pp.

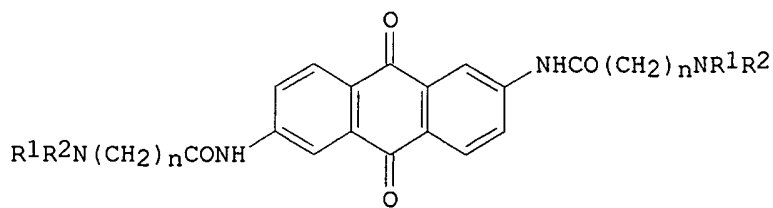
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9100265	A1	19910110	WO 1990-GB1004	19900629
	W: JP, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, IT, LU, NL, SE				
EP	482119	A1	19920429	EP 1990-917804	19900629
	R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, LU, NL, SE				
PRAI	GB 1989-15028		19890630		
	WO 1990-GB1004		19900629		
GI					



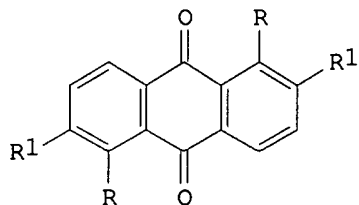
AB The title compds. [I; n = 1, 2, 3; R1, R2 = Et, CH2CH2OH, CH2OH; or R1R2N = piperidino, 2- or 4-(2-hydroxyethyl)piperidino, 2-(hydroxymethyl)piperidino, 4-(2-hydroxyethyl)- or 4-methylpiperidino, morpholino], useful for treating a host suffering from cancer, are prepd. I intercalating into DNA with one side-chain of the mol. residing in each DNA groove, are cytotoxic and non-mutagenic. Thus, a suspension of 14.3 mmol 2,6-bis(3-chloropropionamido)anthracene-9,10-dione in EtOH was gently refluxed and 0.12 mol 4-(2-hydroxyethyl)piperidine in EtOH was added dropwise during 30 min and refluxing was continued for 5 h to give I [n = 2, R1R2N = 4-(2-hydroxyethyl)piperidino] (II). I stabilized various DNA's towards thermal denaturation, the effect of increasing the melting temp. for the DNA by I (n = 2) was comparable to that of mitoxantrone (III) (a known intercalator), and unwinded covalently-colored supercoiled plasmid PM2 DNA. I in vitro showed IC50 of 0.25 - >100 .mu.mol/dm3 against L1210 leukemia cell lines, vs. 0.002 .mu.mol/dm3 with III. II.2AcOH at 200 mg/kg/day i.p. on days 3, 5, 6, and 7 increased 136.8% the life span of mice bearing L1210 leukemia tumor.

REFERENCE 4

AN 113:111062 CA
TI Interaction of "monobasic" anthraquinones with DNA sequences
AU Meister, Walter Vesely; Skoelziger, Regina; Luck, Gerhard; Radtke, Christel; Munsche, Dieter; Witkowski, Werner; Hoffmann, Siegfried
CS Sekt. Chem., Martin-Luther-Univ. Halle-Wittenberg, Halle/Saale, DDR-4010, Ger. Dem. Rep.
SO Zeitschrift fuer Chemie (1990), 30(3), 95-6
CODEN: ZECEAL; ISSN: 0044-2402
DT Journal
LA German
AB The interaction of monobasic 1-hydroxy-9,10-anthracenedione with DNA was examd. by DNA m.p. changes and CD and compared with the 1,5- and 2,6-dibasic 9,10-anthracenediones. The monobasic anthraquinone showed an intermediate effect on melting temp. of chicken DNA compared to the 2 dibasic compds. but showed a similar effect on melting of double-stranded d(A-T)n. This suggests an affinity of the monobasic compd. for GC-rich regions of DNA. The monobasic anthraquinone partially intercalates into the DNA with addnl. electrostatic N-terminal binding.

REFERENCE 5

AN 110:110268 CA
 TI Interactions of "dibasic" anthraquinones with DNA-sequences
 AU Meister, Walter Vesely; Skoelziger, Regina; Luck, Gerhard; Radke, Christel; Munsche, Dieter; Witkowski, Werner; Hoffmann, Siegfried
 CS Sekt. Chem., Martin Luther Univ. Halle-Wittenberg, Halle/Saale, DDR-4010, Ger. Dem. Rep.
 SO Zeitschrift fuer Chemie (1988), 28(9), 331-3
 CODEN: ZECEAL; ISSN: 0044-2402
 DT Journal
 LA German
 GI

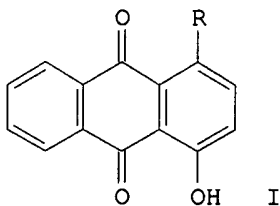


I, $R = \text{NHCOCH}_2\text{NEt}_2$, $R^1 = \text{H}$
 II, $R = \text{H}$, $R^1 = \text{NHCOCH}_2\text{NEt}_2$

AB Two dibasic 9,10-anthracenediones (I and II) show DNA/effector interactions comparable to tilorone and fluoramide intercalators. The DNA/effector interactions were investigated by CD spectrometry and melting-point charge expts. Using chicken DNA, II showed a greater effect on m.p. (ΔT_m I:II, 4.5:23.0), whereas the effects on $[d(A-T)n]$ were similar (ΔT_m I:II, 10.5/13.5). The effects on melting temp. were supported by relative changes in CD spectra resulting from intercalation of the effectors.

REFERENCE 6

AN 106:213557 CA
 TI Mono- and bis-basic anthraquinones
 AU Hoffmann, Siegfried; Skoelziger, Regina; Witkowski, Werner
 CS Sekt. Chem., Martin-Luther-Univ. Halle-Wittenberg, Halle/Saale, DDR-4020, Ger. Dem. Rep.
 SO Zeitschrift fuer Chemie (1986), 26(6), 206-7
 CODEN: ZECEAL; ISSN: 0044-2402
 DT Journal
 LA German
 GI

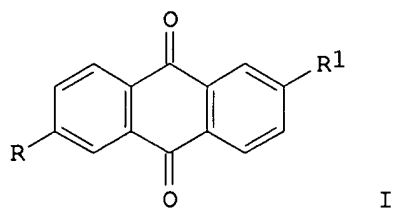


AB Aminohydroxyanthracenedione I ($R = \text{NH}_2$) in PhNO_2 was acylated with ClCH_2COCl to give 89% I ($R = \text{ClCH}_2\text{CONH}$), which was treated with R_1NH_2 ($\text{R}_1 = \text{Et, Pr, Bu}$) to give 29-43% I ($R = \text{R}_1\text{NCH}_2\text{CONH}$). 1,5- And 2,6-diamino-9,10-anthracenediones were similarly prepd.

REFERENCE 7

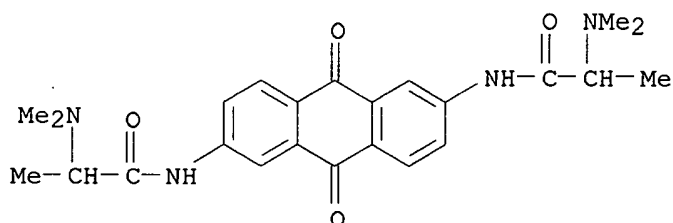
AN 92:110720 CA

TI Chemotherapeutically active anthraquinones. I. Aminoanthraquinones
 AU Winkelmann, E.; Raether, W.
 CS Hoechst A.-G., Frankfurt/Main, D-6230, Fed. Rep. Ger.
 SO Arzneimittel-Forschung (1979), 29(10), 1504-9
 CODEN: ARZNAD; ISSN: 0004-4172
 DT Journal
 LA English
 GI



AB Anthraquinones I (R = R1 = optionally substituted acylamino and alkyleneamino; R = H, R1 = N:CHNMe2; R = R1 = aminoalkyleneamino) (46 compds.) were prepd. by substitution of the corresponding amines by chloroacyl chlorides or amidation of the acylamines. I (R = R1 = aminoalkyleneamino) most effectively controlled *Trichomonas vaginalis*, *T. fetus* and *Entameba histolytica*. Thus, anthraquinone systems and bis(amidino) groups are needed for protozoacidal activity.

L4 ANSWER 40 OF 47 REGISTRY COPYRIGHT 2003 ACS
 RN 62799-47-7 REGISTRY
 CN Propanamide, N,N'-(9,10-dihydro-9,10-dioxo-2,6-anthracenediyl)bis[2-(dimethylamino)- (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C24 H28 N4 O4
 LC STN Files: BEILSTEIN*, CA, CAPLUS
 (*File contains numerically searchable property data)

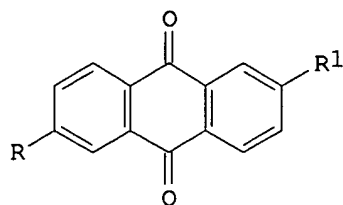


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1957 TO DATE)
 2 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 92:110720 CA
 TI Chemotherapeutically active anthraquinones. I. Aminoanthraquinones
 AU Winkelmann, E.; Raether, W.
 CS Hoechst A.-G., Frankfurt/Main, D-6230, Fed. Rep. Ger.
 SO Arzneimittel-Forschung (1979), 29(10), 1504-9
 CODEN: ARZNAD; ISSN: 0004-4172
 DT Journal
 LA English
 GI



I

AB Anthraquinones I (R = R1 = optionally substituted acylamino and alkyleneamino; R = H, R1 = N:CHNMe2; R = R1 = aminoalkyleneamino) (46 compds.) were prepd. by substitution of the corresponding amines by chloroacyl chlorides or amidation of the acylamines. I (R = R1 = aminoalkyleneamino) most effectively controlled *Trichomonas vaginalis*, *T. fetus* and *Entameba histolytica*. Thus, anthraquinone systems and bis(amidino) groups are needed for protozoacidal activity.

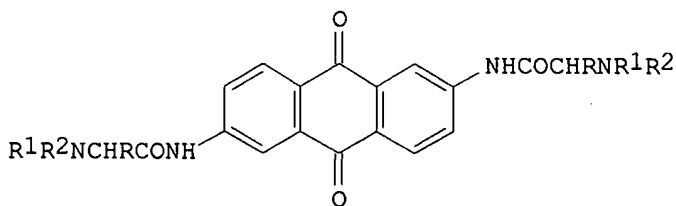
REFERENCE 2

AN 87:5728 CA
 TI Substituted 2,6-diaminoanthraquinones
 IN Winkelmann, Erhardt; Raether, Wolfgang; Rolly, Heinrich
 FA Hoechst A.-G., Fed. Rep. Ger.
 SO Ger. Offen., 11 pp.
 CODEN: GWXXBX

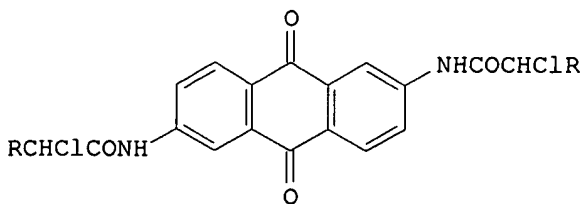
DT Patent
 LA German
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2537878	A1	19770310	DE 1975-2537878	19750826
	NL 7609285	A	19770301	NL 1976-9285	19760820
	DK 7603846	A	19770227	DK 1976-3846	19760825
	BE 845550	A1	19770228	BE 1976-170105	19760826
	JP 52027759	A2	19770302	JP 1976-101180	19760826
	FR 2321881	A1	19770325	FR 1976-25806	19760826
PRAI	DE 1975-2537878		19750826		

GI



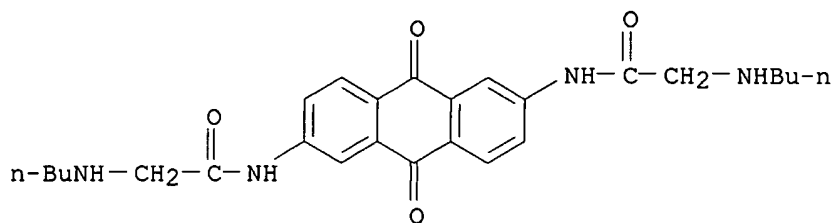
I



II

AB Anthraquinone derivs. I (R, R1 = H, Me; R2 = H, Me, Et, Bu, Me2CH, etc.) were prepd. by the reaction of II (R = H, Me) with NH3 or R1R2NH. I are useful as amebicides and virucides (no data).

RN 62799-46-6 REGISTRY
 CN Acetamide, N,N'-(9,10-dihydro-9,10-dioxo-2,6-anthracenediyl)bis[2-(butylamino)- (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C26 H32 N4 O4
 LC STN Files: BEILSTEIN*, CA, CAPLUS
 (*File contains numerically searchable property data)

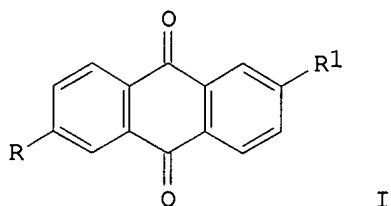


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1957 TO DATE)
 2 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 92:110720 CA
 TI Chemotherapeutically active anthraquinones. I. Aminoanthraquinones
 AU Winkelmann, E.; Raether, W.
 CS Hoechst A.-G., Frankfurt/Main, D-6230, Fed. Rep. Ger.
 SO Arzneimittel-Forschung (1979), 29(10), 1504-9
 CODEN: ARZNAD; ISSN: 0004-4172
 DT Journal
 LA English
 GI

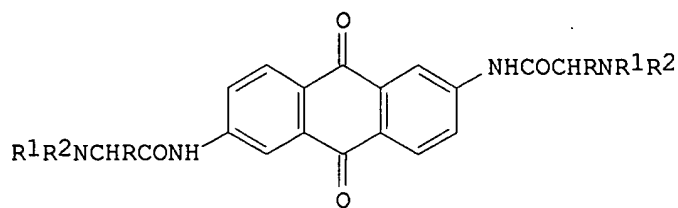


AB Anthraquinones I (R = R1 = optionally substituted acylamino and alkyleneamino; R = H, R1 = N:CHNMe2; R = R1 = aminoalkyleneamino) (46 compds.) were prepd. by substitution of the corresponding amines by chloroacyl chlorides or amidation of the acylamines. I (R = R1 = aminoalkyleneamino) most effectively controlled *Trichomonas vaginalis*, *T. fetus* and *Entameba histolytica*. Thus, anthraquinone systems and bis(amidino) groups are needed for protozoacidal activity.

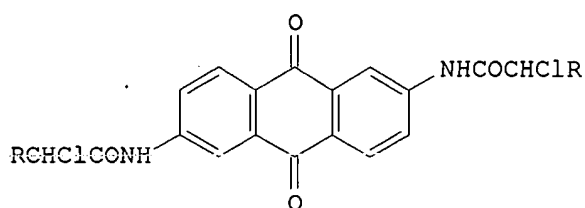
REFERENCE 2

AN 87:5728 CA
 TI Substituted 2,6-diaminoanthraquinones
 IN Winkelmann, Erhardt; Raether, Wolfgang; Rolly, Heinrich
 PA Hoechst A.-G., Fed. Rep. Ger.
 SO Ger. Offen., 11 pp.
 CODEN: GWXXBX
 DT Patent
 LA German
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2537878	A1	19770310	DE 1975-2537878	19750826
	NL 7609285	A	19770301	NL 1976-9285	19760820
	DK 7603846	A	19770227	DK 1976-3846	19760825
	BE 845550	A1	19770228	BE 1976-170105	19760826
	JP 52027759	A2	19770302	JP 1976-101180	19760826
	FR 2321881	A1	19770325	FR 1976-25806	19760826
PRAI	DE 1975-2537878		19750826		
GI					



I



II

AB Anthraquinone derivs. I ($R, R^1 = H, Me; R^2 = H, Me, Et, Bu, Me_2CH$, etc.) were prepd. by the reaction of II ($R = H, Me$) with NH_3 or R^1R^2NH . I are useful as amebicides and virucides (no data).

L4 ANSWER 42 OF 47 REGISTRY COPYRIGHT 2003 ACS

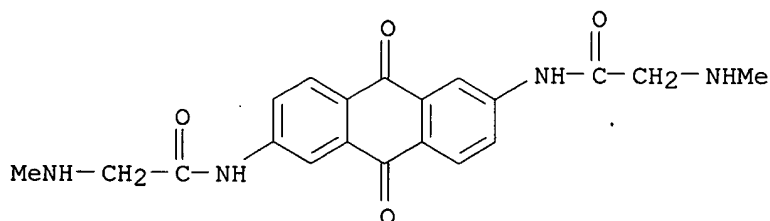
RN 62799-45-5 REGISTRY

CN Acetamide, N,N'-(9,10-dihydro-9,10-dioxo-2,6-anthracenediyl)bis[2-(methylamino)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C20 H20 N4 O4

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1957 TO DATE)

2 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 105:146232 CA

TI Immunoactive compounds.

IN Biber, Rudolf

PA Austria

SO PCT Int. Appl., 12 pp.

CODEN: PIXXD2

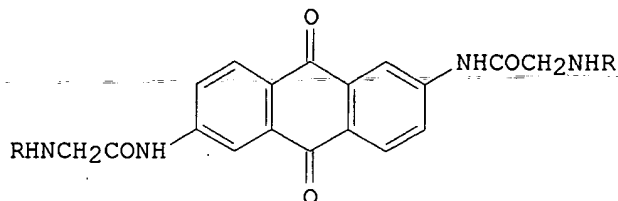
DT Patent

LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 8600892	A1	19860213	WO 1985-AT19	19850731
	W: AU, BG, BR, CH, DE, DK, FI, GB, HU, JP, NL, NO, RO, SE, SU, US				
	RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
	AU 8546799	A1	19860225	AU 1985-46799	19850731
	EP 191058	A1	19860820	EP 1985-903971	19850731
	EP 191058	B1	19890329		
	R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
	HU 39150	A2	19860828	HU 1985-3770	19850731
	HU 197511	B	19890428		
	JP 61502891	T2	19861211	JP 1985-503498	19850731
	JP 05072903	B4	19931013		
	AT 41769	E	19890415	AT 1985-903971	19850731
	US 4794125	A	19881227	US 1988-186688	19880421
PRAI	AT 1984-2468		19840801		
	EP 1985-903971		19850731		
	WO 1985-AT19		19850731		
	US 1986-862355		19860530		

GI



I

AB The anthraquinones I (R = lower alkyl) are prepd. as immunoactive agents and neoplasm inhibitors. Thus, a mixt. of 2,6-bis(chloroacetyl-amino)anthraquinone, MeNH₂ and EtOH was heated at 80.degree. for 3 h to give I (R = Me) (II). In the delayed hypersensitivity test in mice (Dietrich, F. M. and Hess, R., 1970), II was much more immunosuppressant than the std. cyclosporin A.

REFERENCE 2

AN 87:5728 CA
 TI Substituted 2,6-diaminoanthraquinones
 IN Winkelmann, Erhardt; Raether, Wolfgang; Rolly, Heinrich
 PA Hoechst A.-G., Fed. Rep. Ger.
 SO Ger. Offen., 11 pp.
 CODEN: GWXXBX

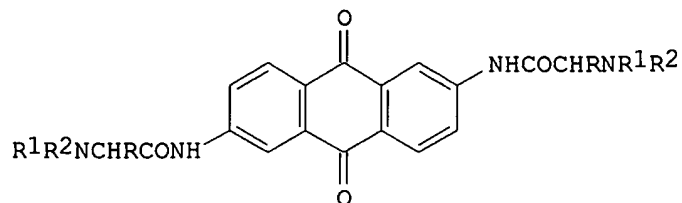
DT Patent

LA German

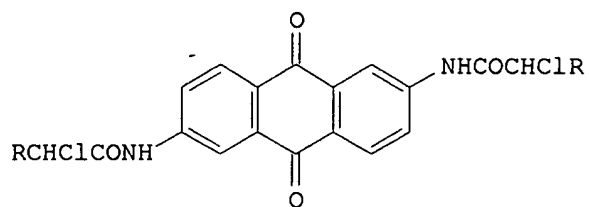
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2537878	A1	19770310	DE 1975-2537878	19750826
	NL 7609285	A	19770301	NL 1976-9285	19760820
	DK 7603846	A	19770227	DK 1976-3846	19760825
	BE 845550	A1	19770228	BE 1976-170105	19760826
	JP 52027759	A2	19770302	JP 1976-101180	19760826
	FR 2321881	A1	19770325	FR 1976-25806	19760826
PRAI	DE 1975-2537878		19750826		

GI



I



II

AB Anthraquinone derivs. I (R, R1 = H, Me; R2 = H, Me, Et, Bu, Me2CH, etc.) were prepd. by the reaction of II (R = H, Me) with NH3 or R1R2NH. I are useful as amebicides and virucides (no data).

L4 ANSWER 43 OF 47 REGISTRY COPYRIGHT 2003 ACS

RN 62799-44-4 REGISTRY

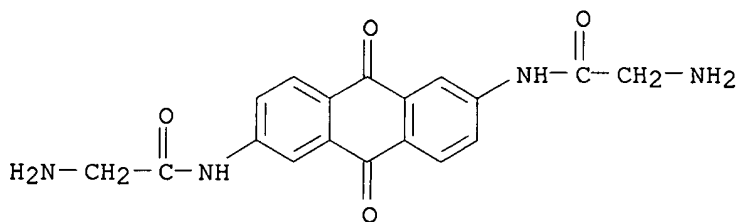
CN Acetamide, N,N'-(9,10-dihydro-9,10-dioxo-2,6-anthracenediyl)bis(2-amino-

(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C18 H16 N4 O4

LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)

1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

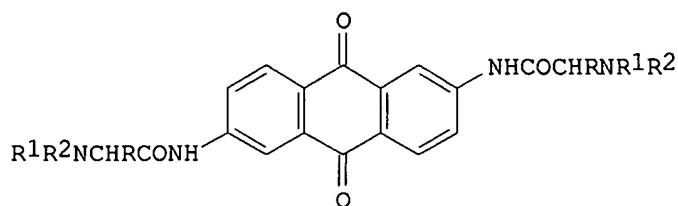
AN 87:5728 CA
 TI Substituted 2,6-diaminoanthraquinones
 IN Winkelmann, Erhardt; Raether, Wolfgang; Rolly, Heinrich
 PA Hoechst A.-G., Fed. Rep. Ger.
 SO Ger. Offen., 11 pp.
 CODEN: GWXXBX

DT Patent

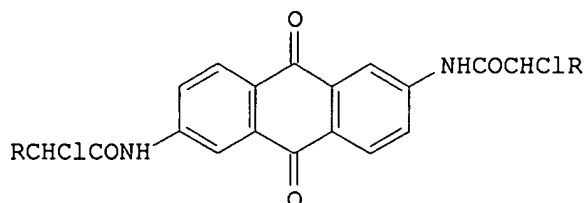
LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2537878	A1	19770310	DE 1975-2537878	19750826
	NL 7609285	A	19770301	NL 1976-9285	19760820
	DK 7603846	A	19770227	DK 1976-3846	19760825
	BE 845550	A1	19770228	BE 1976-170105	19760826
	JP 52027759	A2	19770302	JP 1976-101180	19760826



I



II

AB Anthraquinone derivs. I (R, R1 = H, Me; R2 = H, Me, Et, Bu, Me2CH, etc.) were prep'd. by the reaction of II (R = H, Me) with NH3 or R1R2NH. I are useful as amebicides and virucides (no data).

L4 ANSWER 44 OF 47 REGISTRY COPYRIGHT 2003 ACS

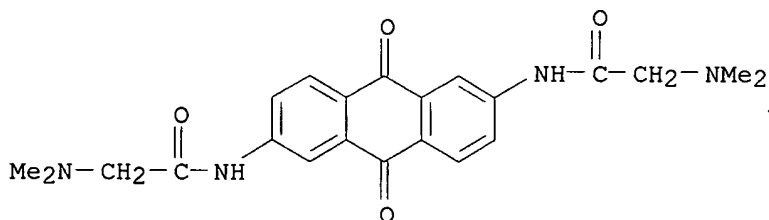
RN 62799-43-3 REGISTRY

CN Acetamide, N,N'-(9,10-dihydro-9,10-dioxo-2,6-anthracenediyl)bis[2-(dimethylamino)-, dihydrochloride (9CI) (CA INDEX NAME)

MF C22 H24 N4 O4 . 2 Cl H

LC STN Files: CA, CAPLUS, CHEMCATS

CRN (62799-42-2)

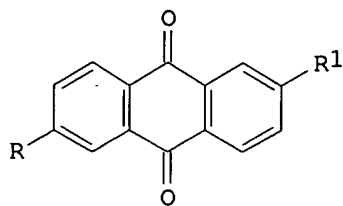


● 2 HCl

2 REFERENCES IN FILE CA (1957 TO DATE)
 2 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 92:110720 CA
 TI Chemotherapeutically active anthraquinones. I. Aminoanthraquinones
 AU Winkelmann, E.; Raether, W.
 CS Hoechst A.-G., Frankfurt/Main, D-6230, Fed. Rep. Ger.
 SO Arzneimittel-Forschung (1979), 29(10), 1504-9
 CODEN: ARZNAD; ISSN: 0004-4172
 DT Journal
 LA English
 GI



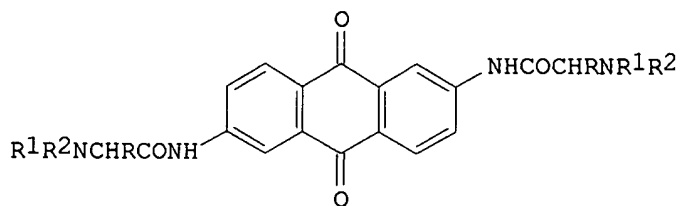
I

AB Anthraquinones I (R = R1 = optionally substituted acylamino and alkyleneamino; R = H, R1 = N:CHNMe2; R = R1 = aminoalkyleneamino) (46 compds.) were prepd. by substitution of the corresponding amines by chloroacyl chlorides or amidation of the acylamines. I (R = R1 = aminoalkyleneamino) most effectively controlled *Trichomonas vaginalis*, *T. fetus* and *Entameba histolytica*. Thus, anthraquinone systems and bis(amidino) groups are needed for protozoacidal activity.

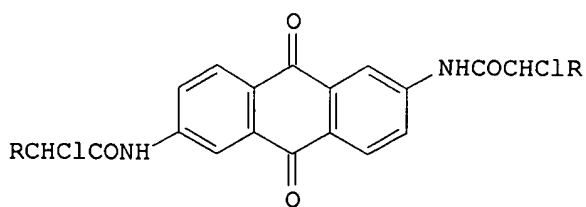
REFERENCE 2

AN 87:5728 CA
 TI Substituted 2,6-diaminoanthraquinones
 IN Winkelmann, Erhardt; Raether, Wolfgang; Rolly, Heinrich
 PA Hoechst A.-G., Fed. Rep. Ger.
 SO Ger. Offen., 11 pp.
 CODEN: GWXXBX
 DT Patent
 LA German
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2537878	A1	19770310	DE 1975-2537878	19750826
	NL 7609285	A	19770301	NL 1976-9285	19760820
	DK 7603846	A	19770227	DK 1976-3846	19760825
	BE 845550	A1	19770228	BE 1976-170105	19760826
	JP 52027759	A2	19770302	JP 1976-101180	19760826
	FR 2321881	A1	19770325	FR 1976-25806	19760826
PRAI	DE 1975-2537878		19750826		
GI					



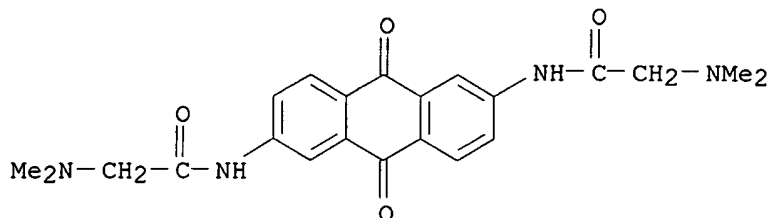
I



II

AB Anthraquinone derivs. I (R, R1 = H, Me; R2 = H, Me, Et, Bu, Me2CH, etc.) were prepd. by the reaction of II (R = H, Me) with NH3 or R1R2NH. I are useful as amebicides and virucides (no data).

RN 62799-42-2 REGISTRY
 CN Acetamide, N,N'-(9,10-dihydro-9,10-dioxo-2,6-anthracenediyl)bis[2-(dimethylamino)- (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C22 H24 N4 O4
 CI COM
 LC STN Files: BEILSTEIN*, CA, CAPLUS
 (*File contains numerically searchable property data)

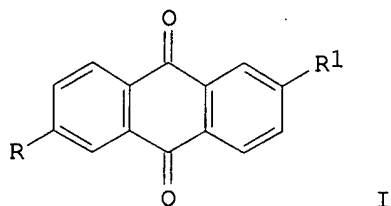


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1957 TO DATE)
 3 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 92:110720 CA
 TI Chemotherapeutically active anthraquinones. I. Aminoanthraquinones
 AU Winkelmann, E.; Raether, W.
 CS Hoechst A.-G., Frankfurt/Main, D-6230, Fed. Rep. Ger.
 SO Arzneimittel-Forschung (1979), 29(10), 1504-9
 CODEN: ARZNAD; ISSN: 0004-4172
 DT Journal
 LA English
 GI



AB Anthraquinones I (R = R1 = optionally substituted acylamino and alkyleneamino; R = H, R1 = N:CHNMe2; R = R1 = aminoalkyleneamino) (46 compds.) were prepd. by substitution of the corresponding amines by chloroacyl chlorides or amidation of the acylamines. I (R = R1 = aminoalkyleneamino) most effectively controlled *Trichomonas vaginalis*, *T. fetus* and *Entameba histolytica*. Thus, anthraquinone systems and bis(amidino) groups are needed for protozoacidal activity.

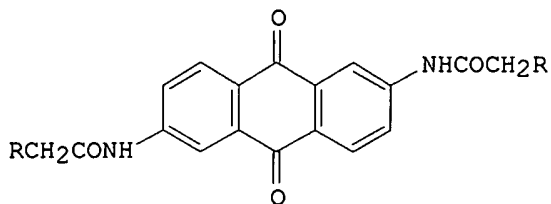
REFERENCE 2

AN 88:37503 CA
 TI 2,6-Bis(aminoacylamino)anthraquinones and their acid addition salts with antiviral and interferon-inducing properties
 IN Biber, Rudolf
 PA Austria
 SO Ger. Offen., 6 pp.
 CODEN: GWXXBX
 DT Patent

LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2702137	A1	19770929	DE 1977-2702137	19770120
	AT 7600399	A	19771015	AT 1976-399	19760122
	AT 351521	B	19790725		
PRAI	AT 1976-399		19760122		
GI					



I

AB The title compds. I (R = NMe₂, hexamethylenimino) were prepd., e.g., by refluxing a mixt. of I (R = Cl), HNMe₂, EtOH, and DMF 2 h. I were used in treating virus infections at 250-500 mg per dose.

REFERENCE 3

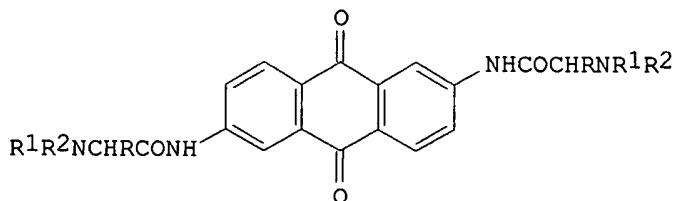
AN 87:5728 CA
 TI Substituted 2,6-diaminoanthraquinones
 IN Winkelmann, Erhardt; Raether, Wolfgang; Rolly, Heinrich
 PA Hoechst A.-G., Fed. Rep. Ger.
 SO Ger. Offen., 11 pp.
 CODEN: GWXXBX

DT Patent

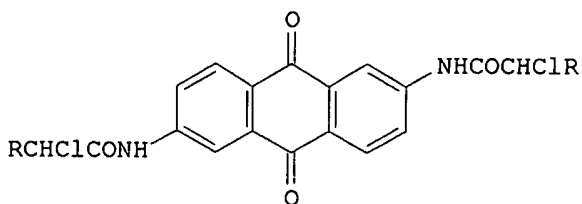
LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2537878	A1	19770310	DE 1975-2537878	19750826
	NL 7609285	A	19770301	NL 1976-9285	19760820
	DK 7603846	A	19770227	DK 1976-3846	19760825
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	JP 52027759	A2	19770302	JP 1976-101180	19760826
	FR 2321881	A1	19770325	FR 1976-25806	19760826
PRAI	DE 1975-2537878		19750826		
GI					



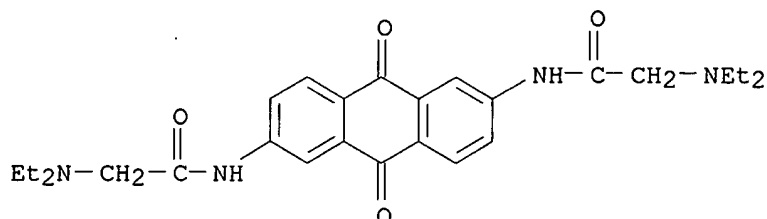
I



II

AB Anthraquinone derivs. I (R, R1 = H, Me; R2 = H, Me, Et, Bu, Me2CH, etc.) were prepd. by the reaction of II (R = H, Me) with NH3 or R1R2NH. I are useful as amebicides and virucides (no data).

L4 ANSWER 46 OF 47 REGISTRY COPYRIGHT 2003 ACS
 RN 55077-14-0 REGISTRY
 CN Acetamide, N,N'-(9,10-dihydro-9,10-dioxo-2,6-anthracenediyl)bis[2-(diethylamino)-, dihydrochloride (9CI) (CA INDEX NAME)
 MF C26 H32 N4 O4 . 2 Cl H
 LC STN Files: CA, CAPLUS, USPATFULL
 CRN (72966-57-5)



●2 HCl

1 REFERENCES IN FILE CA (1957 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

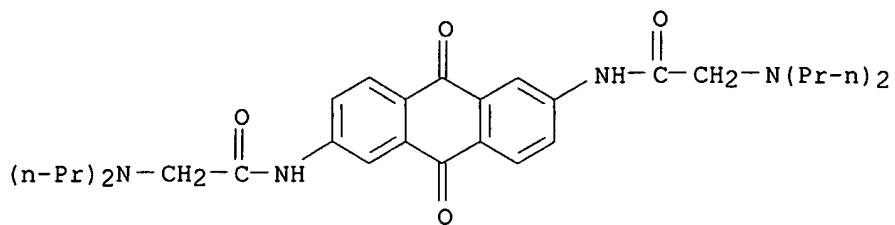
AN 82:139857 CA
 TI Disubstituted acetamidoanthraquinones
 IN Santilli, Arthur A.; Scoiese, Anthony C.; Bell, Stanley C.
 PA American Home Products Corp.
 SO U.S., 3 pp.
 CODEN: USXXAM
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3859315	A	19750107	US 1972-302308	19721030
PRAI	US 1972-302308		19721030		

GI For diagram(s), see printed CA Issue.

AB 2,6-Bis(2-chloroacetamido)anthraquinone was aminated to give the following I (R = Pr, Et; NR2 = morpholino) which demonstrated antiinflammatory activity.

L4 ANSWER 47 OF 47 REGISTRY COPYRIGHT 2003 ACS
 RN 55077-13-9 REGISTRY
 CN Acetamide, N,N'-(9,10-dihydro-9,10-dioxo-2,6-anthracenediyl)bis[2-(dipropylamino)-, dihydrochloride (9CI) (CA INDEX NAME)
 MF C30 H40 N4 O4 . 2 Cl H
 LC STN Files: CA, CAPLUS, USPATFULL
 CRN (108428-64-4)



●2 HCl

1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1

AN 82:139857 CA
TI Disubstituted acetamidoanthraquinones
IN Santilli, Arthur A.; Scoïese, Anthony C.; Bell, Stanley C.
PA American Home Products Corp.
SO U.S., 3 pp.
CODEN: USXXAM

DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3859315	A	19750107	US 1972-302308	19721030
PRAI	US 1972-302308		19721030		

GI For diagram(s), see printed CA Issue.
AB 2,6-Bis(2-chloroacetamido)anthraquinone was aminated to give the following
I (R = Pr, Et; NR2 = morpholino) which demonstrated antiinflammatory
activity.

=>